



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 AM GMT

PDB ID : 2X0B
Title : CRYSTAL STRUCTURE OF HUMAN ANGIOTENSINOGEN COM-
PLEXED WITH RENIN
Authors : Zhou, A.; Wei, Z.; Yan, Y.; Carrell, R.W.; Read, R.J.
Deposited on : 2009-12-08
Resolution : 4.33 Å(reported)

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

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

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

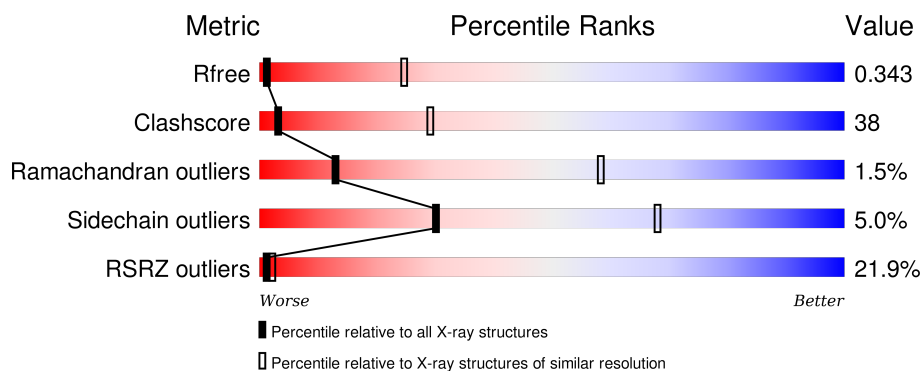
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1063 (5.08-3.60)
Clashscore	102246	1171 (5.08-3.60)
Ramachandran outliers	100387	1110 (5.08-3.60)
Sidechain outliers	100360	1093 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	383	<div> <div>9%</div> <div>55%</div> <div>29%</div> <div>•</div> <div>14%</div> </div>
1	C	383	<div> <div>15%</div> <div>55%</div> <div>30%</div> <div>•</div> <div>14%</div> </div>
1	E	383	<div> <div>15%</div> <div>56%</div> <div>28%</div> <div>•</div> <div>14%</div> </div>
1	G	383	<div> <div>14%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>14%</div> </div>
2	B	452	<div> <div>18%</div> <div>52%</div> <div>37%</div> <div>•</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	452	<div><div></div><div>32%</div><div>53%</div><div>36%</div><div>6%</div></div>
2	F	452	<div><div></div><div>20%</div><div>52%</div><div>37%</div><div>6%</div></div>
2	H	452	<div><div></div><div>32%</div><div>53%</div><div>36%</div><div>6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23244 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	C	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	E	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	G	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			

- Molecule 2 is a protein called ANGIOTENSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	D	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	F	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	H	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			

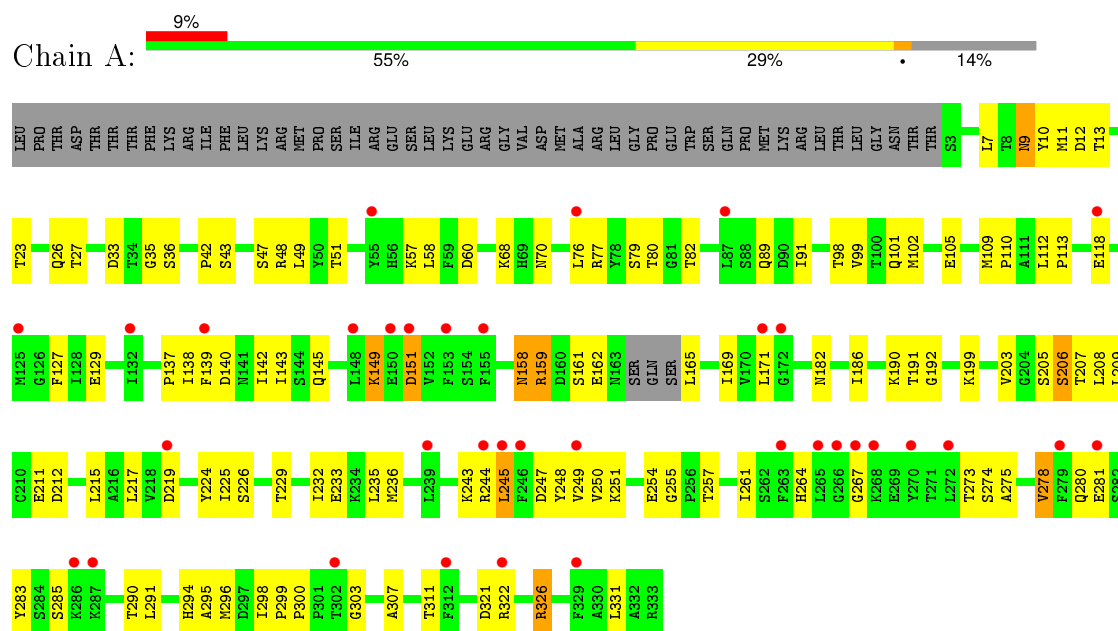
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ASN	ASP	CONFLICT	UNP P01019
D	47	ASN	ASP	CONFLICT	UNP P01019
F	47	ASN	ASP	CONFLICT	UNP P01019
H	47	ASN	ASP	CONFLICT	UNP P01019

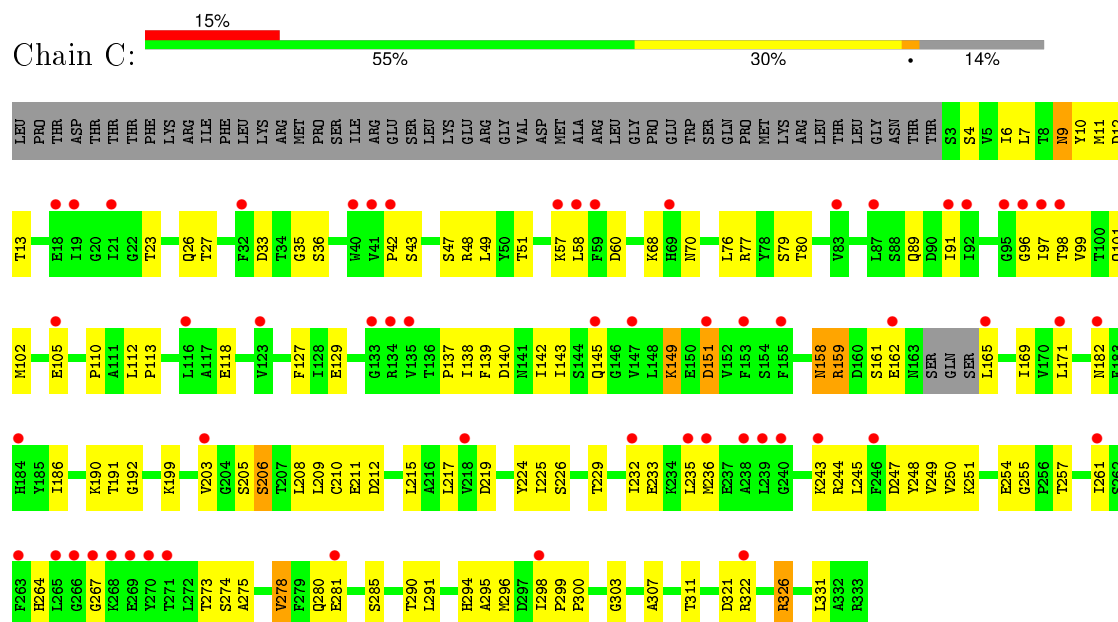
3 Residue-property plots

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

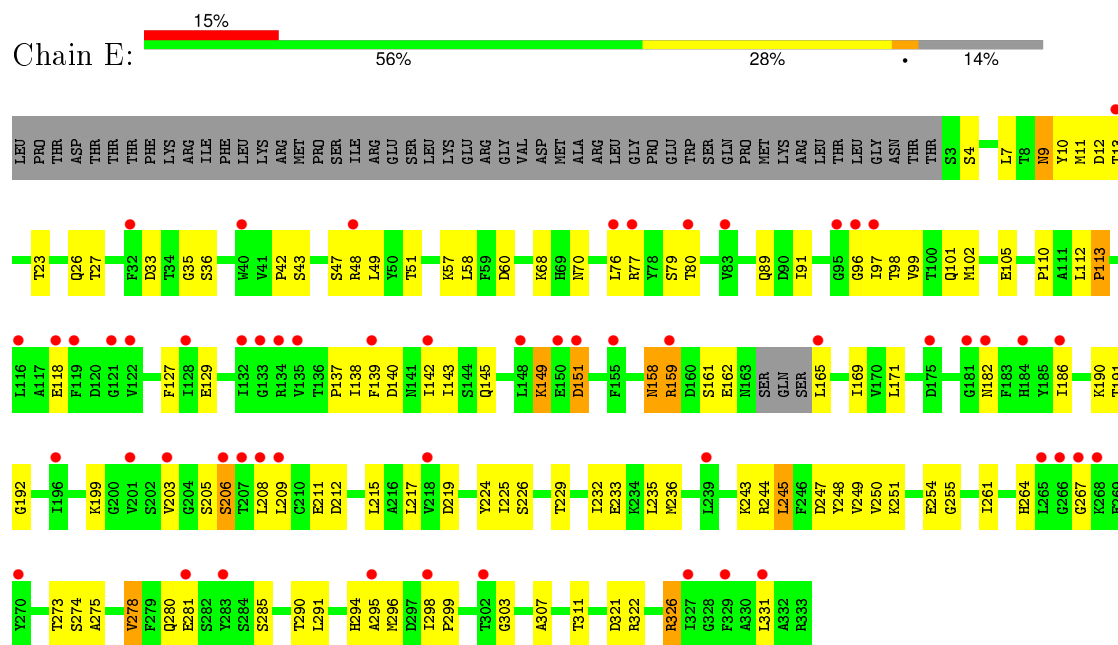
● Molecule 1: RENIN



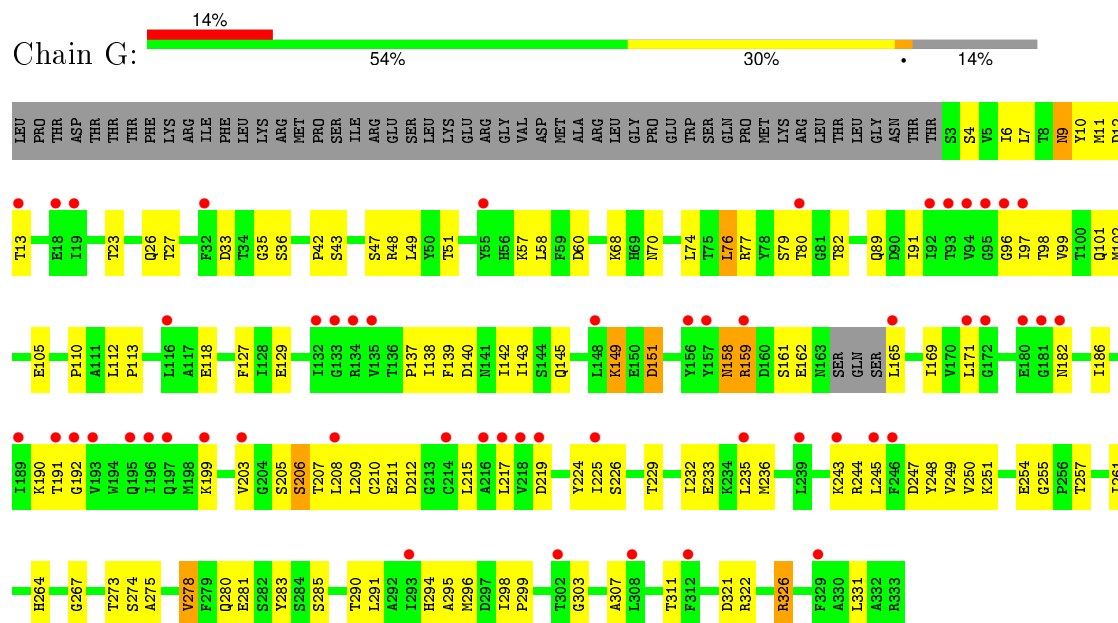
● Molecule 1: RENIN



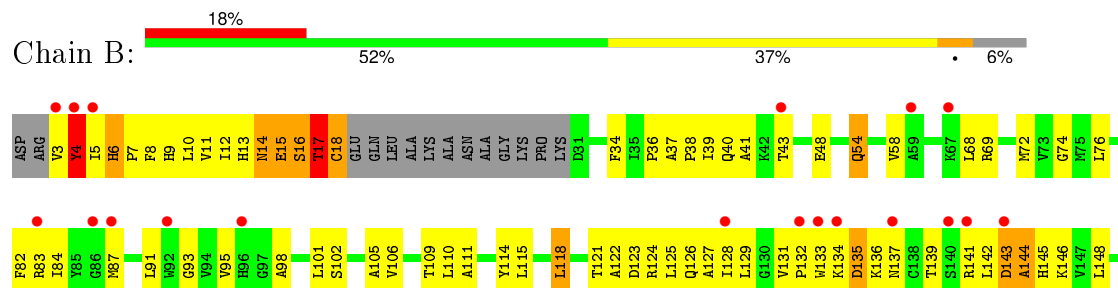
- Molecule 1: RENIN

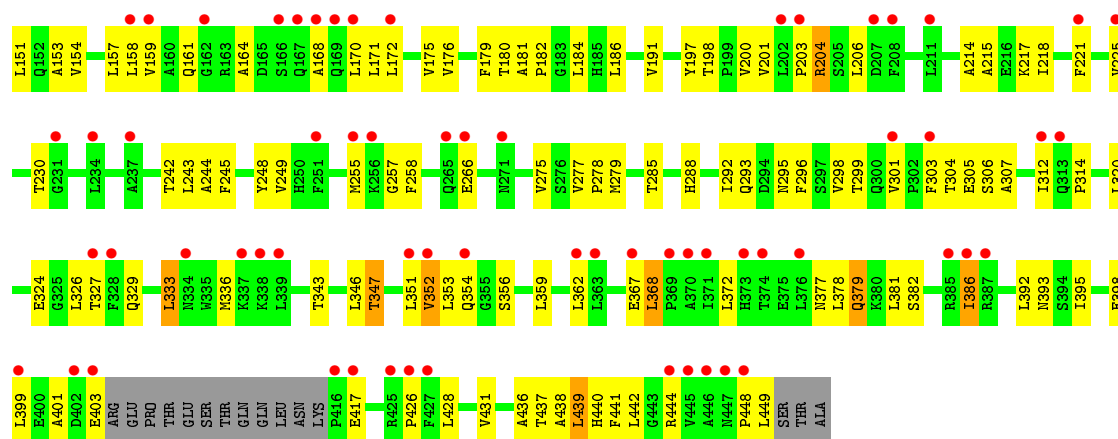


- Molecule 1: RENIN

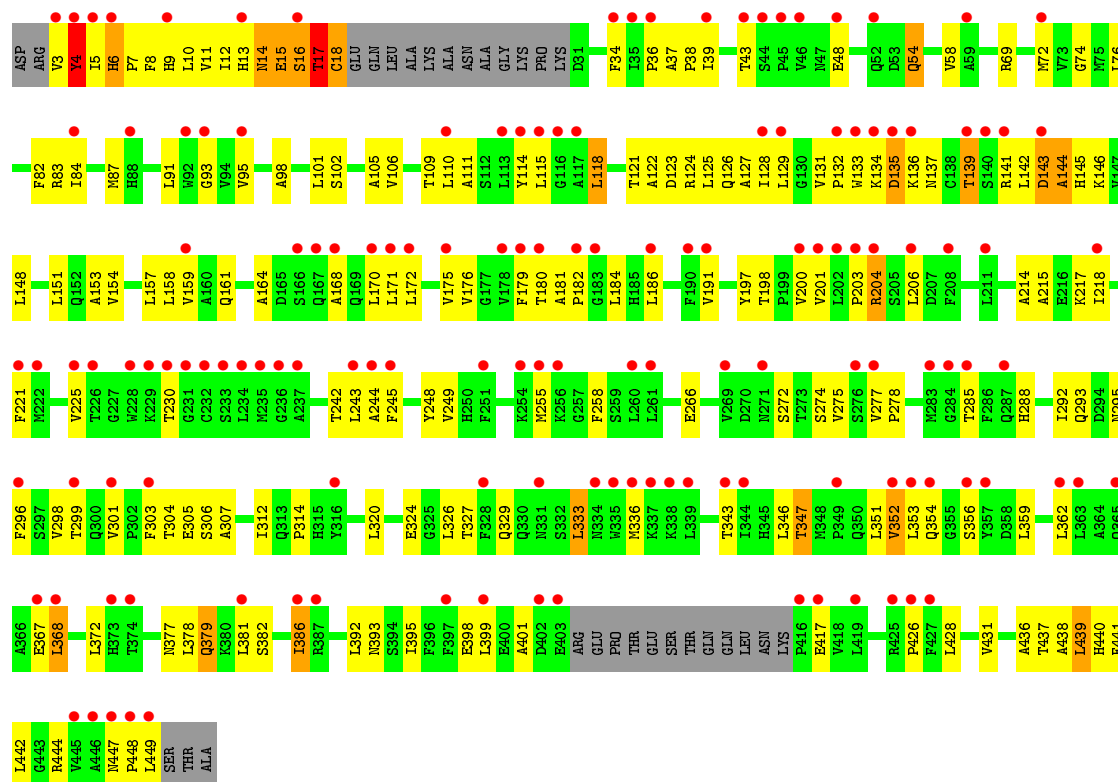


- Molecule 2: ANGIOTENSINOGEN

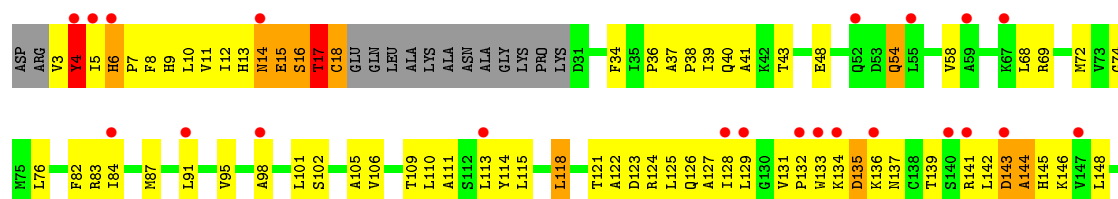


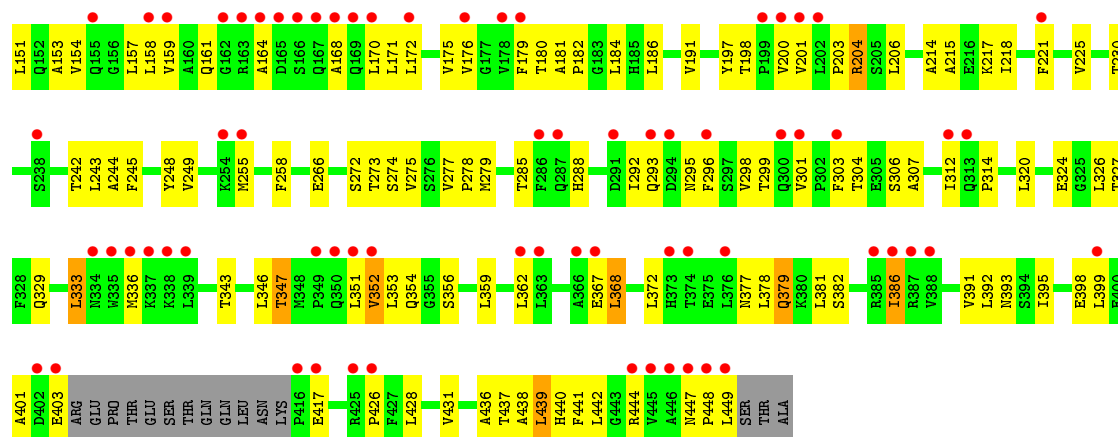


• Molecule 2: ANGIOTENSINOGEN

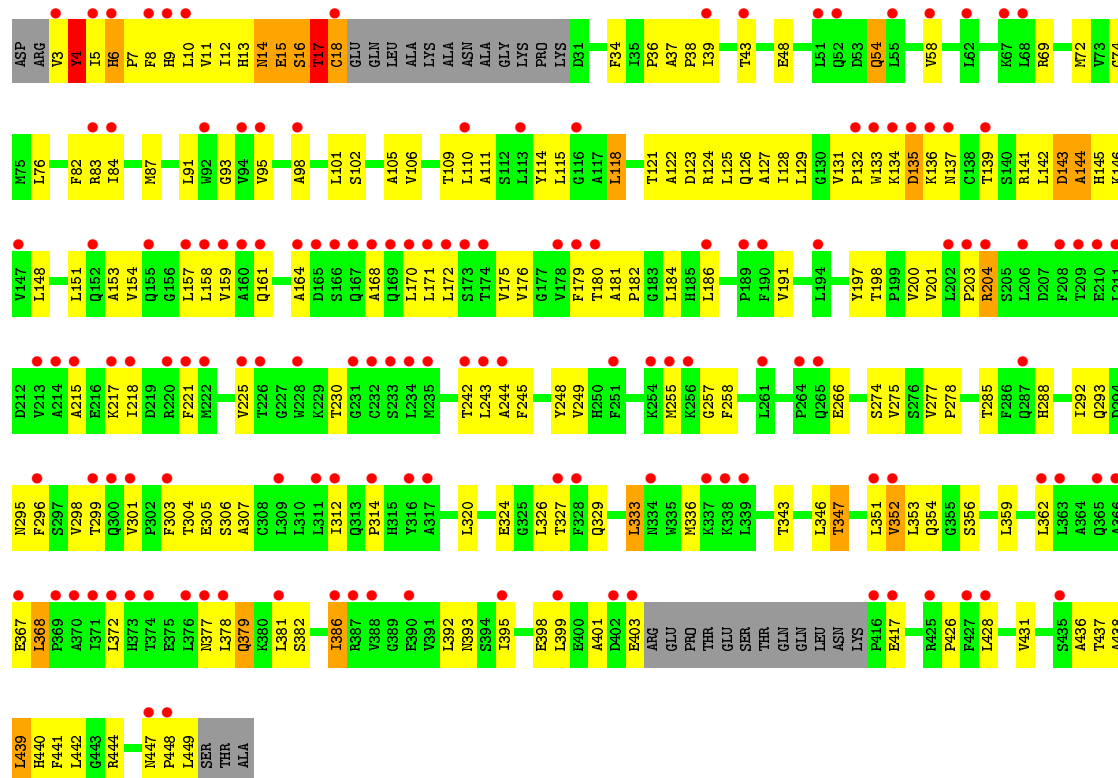


• Molecule 2: ANGIOTENSINOGEN





• Molecule 2: ANGIOTENSINOGEN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	212.47Å 212.47Å 474.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 4.33 48.52 – 4.34	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.52-4.33) 84.2 (48.52-4.34)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 4.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_249)	Depositor
R, R_{free}	0.309 , 0.334 0.326 , 0.343	Depositor DCC
R_{free} test set	2253 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	200.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 44561 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å ²)	325.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/2599	0.67	0/3523
1	C	0.35	0/2599	0.67	0/3523
1	E	0.35	0/2599	0.67	0/3523
1	G	0.35	0/2599	0.67	0/3523
2	B	0.31	0/3345	0.51	5/4557 (0.1%)
2	D	0.31	0/3345	0.51	5/4557 (0.1%)
2	F	0.31	0/3345	0.51	5/4557 (0.1%)
2	H	0.31	0/3345	0.51	5/4557 (0.1%)
All	All	0.33	0/23776	0.59	20/32320 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	PHE	CZ-CE2-CD2	6.16	127.50	120.10
2	F	8	PHE	CZ-CE2-CD2	6.13	127.45	120.10
2	B	8	PHE	CZ-CE2-CD2	6.12	127.44	120.10
2	D	8	PHE	CZ-CE2-CD2	6.08	127.39	120.10
2	H	8	PHE	CG-CD1-CE1	5.27	126.60	120.80
2	B	8	PHE	CG-CD1-CE1	5.26	126.58	120.80
2	F	135	ASP	CB-CG-OD2	5.26	123.03	118.30
2	H	6	HIS	CA-CB-CG	-5.22	104.72	113.60
2	F	8	PHE	CG-CD1-CE1	5.20	126.53	120.80
2	D	8	PHE	CG-CD1-CE1	5.20	126.52	120.80
2	H	135	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	6	HIS	CA-CB-CG	-5.19	104.77	113.60
2	F	6	HIS	CA-CB-CG	-5.19	104.78	113.60
2	F	143	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	135	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	6	HIS	CA-CB-CG	-5.17	104.81	113.60
2	D	135	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	143	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	143	ASP	CB-CG-OD2	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ASP	CB-CG-OD2	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2540	0	2471	198	3
1	C	2540	0	2471	232	2
1	E	2540	0	2470	199	0
1	G	2540	0	2472	227	0
2	B	3271	0	3268	331	28
2	D	3271	0	3268	348	0
2	F	3271	0	3268	360	27
2	H	3271	0	3267	365	0
All	All	23244	0	22955	1748	30

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 38.

All (1748) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:CB	2:D:83:ARG:HH11	1.23	1.49
2:D:142:LEU:CD1	2:D:146:LYS:HE3	1.47	1.45
2:H:142:LEU:CD1	2:H:146:LYS:HE3	1.47	1.43
2:B:142:LEU:CD1	2:B:146:LYS:HE3	1.47	1.42
2:F:142:LEU:CD1	2:F:146:LYS:HE3	1.47	1.42
1:C:98:THR:N	2:F:449:LEU:HD21	1.35	1.35
2:D:131:VAL:HG13	2:D:132:PRO:CA	1.57	1.34
2:F:142:LEU:HD12	2:F:146:LYS:CE	1.56	1.34
2:F:131:VAL:HG13	2:F:132:PRO:CA	1.57	1.33
2:D:142:LEU:HD12	2:D:146:LYS:CE	1.57	1.33
2:B:142:LEU:HD12	2:B:146:LYS:CE	1.56	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:VAL:HG13	2:B:132:PRO:CA	1.57	1.32
2:H:131:VAL:HG13	2:H:132:PRO:CA	1.58	1.32
2:D:272:SER:O	1:G:6:ILE:HG13	1.24	1.32
2:H:142:LEU:HD12	2:H:146:LYS:CE	1.56	1.32
1:G:51:THR:OG1	2:H:83:ARG:CD	1.77	1.32
1:G:51:THR:OG1	2:H:83:ARG:HD3	1.21	1.31
1:E:98:THR:N	2:H:449:LEU:HD21	1.44	1.29
1:E:4:SER:OG	2:H:274:SER:OG	1.52	1.27
2:D:3:VAL:HB	2:D:4:TYR:CD2	1.69	1.26
1:E:51:THR:CB	2:F:83:ARG:HH11	1.47	1.26
2:B:3:VAL:HB	2:B:4:TYR:CD2	1.69	1.26
2:F:3:VAL:HB	2:F:4:TYR:CD2	1.69	1.26
2:H:3:VAL:HB	2:H:4:TYR:CD2	1.69	1.25
1:G:51:THR:CB	2:H:83:ARG:HH11	1.49	1.24
2:D:449:LEU:HD21	1:G:98:THR:N	1.51	1.24
1:C:96:GLY:O	2:F:449:LEU:HD22	1.10	1.24
1:E:51:THR:CG2	2:F:83:ARG:CG	2.14	1.22
1:E:35:GLY:O	2:F:12:ILE:HG22	1.39	1.21
1:C:51:THR:CB	2:D:83:ARG:NH1	1.98	1.21
1:C:97:ILE:C	2:F:449:LEU:HD21	1.60	1.21
1:C:35:GLY:O	2:D:12:ILE:HG22	1.39	1.20
1:A:35:GLY:O	2:B:12:ILE:HG22	1.39	1.20
1:E:23:THR:CG2	2:H:95:VAL:HG21	1.72	1.20
1:C:51:THR:CG2	2:D:83:ARG:HG3	1.71	1.19
1:C:51:THR:HG23	2:D:83:ARG:CG	1.69	1.19
1:E:51:THR:CG2	2:F:83:ARG:HG3	1.72	1.18
1:G:51:THR:CB	2:H:83:ARG:HD3	1.73	1.18
1:A:51:THR:CG2	2:B:83:ARG:CG	2.20	1.17
1:G:35:GLY:O	2:H:12:ILE:HG22	1.39	1.16
1:C:51:THR:CG2	2:D:83:ARG:CG	2.21	1.16
2:F:131:VAL:HG13	2:F:132:PRO:CB	1.75	1.15
2:B:131:VAL:HG13	2:B:132:PRO:CB	1.75	1.15
2:D:131:VAL:HG13	2:D:132:PRO:CB	1.75	1.15
1:A:51:THR:HG21	2:B:83:ARG:HG3	1.16	1.15
1:C:110:PRO:HB3	2:D:132:PRO:HD2	1.26	1.15
1:C:23:THR:HG23	2:F:95:VAL:HG21	1.20	1.15
2:F:126:GLN:CA	2:F:131:VAL:HG21	1.78	1.14
2:H:131:VAL:HG13	2:H:132:PRO:CB	1.75	1.14
2:B:126:GLN:CA	2:B:131:VAL:HG21	1.78	1.14
2:D:131:VAL:HG13	2:D:132:PRO:HA	1.22	1.13
1:C:97:ILE:HA	2:F:449:LEU:CD1	1.79	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:GLN:CA	2:D:131:VAL:HG21	1.78	1.12
2:H:126:GLN:CA	2:H:131:VAL:HG21	1.78	1.12
1:E:112:LEU:HD22	2:F:76:LEU:HD21	1.28	1.12
2:B:131:VAL:HG13	2:B:132:PRO:HA	1.22	1.12
1:E:49:LEU:HD13	2:F:367:GLU:HG3	1.11	1.11
1:E:51:THR:HG23	2:F:83:ARG:HG2	1.30	1.10
1:C:51:THR:HG21	2:D:83:ARG:HG3	1.22	1.10
2:F:131:VAL:HG13	2:F:132:PRO:HA	1.22	1.10
1:E:51:THR:HG23	2:F:83:ARG:CG	1.75	1.10
2:D:126:GLN:HA	2:D:131:VAL:HG21	1.32	1.10
1:A:110:PRO:HB3	2:B:132:PRO:HD2	1.15	1.10
2:B:126:GLN:O	2:B:131:VAL:HG23	1.51	1.10
1:G:110:PRO:CB	2:H:135:ASP:OD1	2.00	1.10
1:C:23:THR:HG23	2:F:95:VAL:CG2	1.81	1.10
2:H:131:VAL:CG1	2:H:132:PRO:CA	2.30	1.09
2:F:126:GLN:O	2:F:131:VAL:HG23	1.51	1.09
2:B:126:GLN:HA	2:B:131:VAL:HG21	1.32	1.09
2:B:131:VAL:CG1	2:B:132:PRO:CA	2.30	1.09
2:F:131:VAL:CG1	2:F:132:PRO:CA	2.30	1.09
1:G:51:THR:OG1	2:H:83:ARG:CZ	2.01	1.08
1:C:49:LEU:HD13	2:D:367:GLU:HG3	1.28	1.08
2:D:131:VAL:CG1	2:D:132:PRO:CA	2.30	1.08
1:A:112:LEU:HD22	2:B:76:LEU:CD2	1.82	1.08
2:H:131:VAL:HG13	2:H:132:PRO:HA	1.22	1.08
2:D:126:GLN:O	2:D:131:VAL:HG23	1.51	1.07
1:E:51:THR:HG21	2:F:83:ARG:HG3	1.10	1.07
2:D:95:VAL:HG21	1:G:23:THR:HG23	1.36	1.07
2:H:126:GLN:O	2:H:131:VAL:HG23	1.51	1.07
1:G:51:THR:OG1	2:H:83:ARG:NE	1.86	1.07
1:C:51:THR:HB	2:D:83:ARG:HH11	1.13	1.07
2:H:131:VAL:CG1	2:H:132:PRO:HB3	1.85	1.07
2:F:131:VAL:CG1	2:F:132:PRO:HB3	1.85	1.07
1:E:23:THR:HG23	2:H:95:VAL:HG21	1.08	1.07
2:B:131:VAL:CG1	2:B:132:PRO:HB3	1.85	1.06
1:G:51:THR:CB	2:H:83:ARG:NH1	2.17	1.06
1:E:13:THR:HG21	2:F:5:ILE:CG2	1.85	1.06
2:H:126:GLN:HA	2:H:131:VAL:HG21	1.32	1.06
2:F:126:GLN:HA	2:F:131:VAL:HG21	1.32	1.06
1:C:13:THR:HG21	2:D:5:ILE:CG2	1.85	1.06
1:A:13:THR:HG21	2:B:5:ILE:CG2	1.85	1.06
1:G:13:THR:HG21	2:H:5:ILE:CG2	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG21	2:B:83:ARG:CG	1.81	1.06
1:C:96:GLY:O	2:F:449:LEU:CD2	2.02	1.06
1:E:51:THR:HB	2:F:83:ARG:HH11	1.18	1.06
1:G:110:PRO:HB3	2:H:132:PRO:CD	1.86	1.05
2:D:272:SER:O	1:G:6:ILE:CG1	2.04	1.05
2:H:132:PRO:HG2	2:H:135:ASP:CA	1.87	1.05
1:E:23:THR:CG2	2:H:95:VAL:CG2	2.35	1.05
2:D:131:VAL:CG1	2:D:132:PRO:HB3	1.85	1.05
2:F:126:GLN:O	2:F:131:VAL:CG2	2.05	1.05
1:G:112:LEU:HD22	2:H:76:LEU:HD21	1.36	1.05
1:C:110:PRO:CB	2:D:135:ASP:OD1	2.05	1.05
2:B:132:PRO:HG2	2:B:135:ASP:CA	1.87	1.04
2:B:122:ALA:O	2:B:126:GLN:HG3	1.57	1.04
2:B:126:GLN:O	2:B:131:VAL:CG2	2.05	1.04
2:D:126:GLN:O	2:D:131:VAL:CG2	2.05	1.04
2:F:132:PRO:HG2	2:F:135:ASP:CA	1.86	1.04
1:G:51:THR:HG21	2:H:83:ARG:HG3	1.39	1.04
2:D:449:LEU:HD21	1:G:98:THR:H	1.03	1.04
1:C:49:LEU:O	2:D:127:ALA:O	1.76	1.04
1:A:112:LEU:HD22	2:B:76:LEU:HD21	1.10	1.04
2:F:122:ALA:O	2:F:126:GLN:HG3	1.57	1.03
2:H:126:GLN:O	2:H:131:VAL:CG2	2.05	1.03
2:D:132:PRO:HG2	2:D:135:ASP:CA	1.87	1.03
2:H:122:ALA:O	2:H:126:GLN:HG3	1.57	1.02
1:A:49:LEU:HD13	2:B:367:GLU:HG3	1.38	1.02
2:D:122:ALA:O	2:D:126:GLN:HG3	1.57	1.02
1:A:112:LEU:CD2	2:B:76:LEU:HD21	1.90	1.02
2:D:142:LEU:HD11	2:D:146:LYS:HE3	1.42	1.01
2:B:142:LEU:HD11	2:B:146:LYS:HE3	1.42	1.01
1:A:51:THR:CB	2:B:83:ARG:HH11	1.71	1.01
2:B:131:VAL:CG1	2:B:132:PRO:CB	2.39	1.01
1:A:51:THR:HG23	2:B:83:ARG:HG2	1.42	1.01
1:G:110:PRO:CB	2:H:132:PRO:HD2	1.90	1.00
2:B:131:VAL:HG13	2:B:132:PRO:HB3	1.43	1.00
1:C:6:ILE:HG13	2:F:272:SER:O	1.61	1.00
2:D:131:VAL:CG1	2:D:132:PRO:CB	2.39	0.99
1:C:51:THR:OG1	2:D:83:ARG:NH1	1.78	0.99
1:G:110:PRO:HB2	2:H:135:ASP:OD1	1.63	0.99
2:H:126:GLN:HA	2:H:131:VAL:CG2	1.93	0.99
2:F:142:LEU:HD11	2:F:146:LYS:HE3	1.42	0.99
1:E:112:LEU:HD22	2:F:76:LEU:CD2	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:HB3	2:B:132:PRO:CD	1.93	0.98
1:C:112:LEU:HD22	2:D:76:LEU:HD21	1.45	0.98
2:B:126:GLN:HA	2:B:131:VAL:CG2	1.93	0.98
2:D:274:SER:OG	1:G:4:SER:OG	1.80	0.98
2:F:131:VAL:CG1	2:F:132:PRO:CB	2.39	0.98
1:G:51:THR:CG2	2:H:83:ARG:CG	2.40	0.98
1:E:98:THR:H	2:H:449:LEU:CD2	1.76	0.98
1:G:110:PRO:CG	2:H:135:ASP:OD1	2.12	0.98
2:H:131:VAL:HG13	2:H:132:PRO:HB3	1.43	0.98
2:F:126:GLN:HA	2:F:131:VAL:CG2	1.93	0.98
2:D:142:LEU:HD12	2:D:146:LYS:HE3	0.98	0.98
1:G:51:THR:HG23	2:H:83:ARG:CG	1.93	0.98
2:B:142:LEU:HD12	2:B:146:LYS:HE3	0.98	0.97
1:E:110:PRO:HB3	2:F:132:PRO:HD2	1.41	0.97
1:A:51:THR:HG23	2:B:83:ARG:CG	1.90	0.97
1:A:112:LEU:CD2	2:B:76:LEU:CD2	2.40	0.97
2:D:126:GLN:HA	2:D:131:VAL:CG2	1.93	0.97
1:G:51:THR:CG2	2:H:83:ARG:HD3	1.94	0.97
2:H:131:VAL:CG1	2:H:132:PRO:CB	2.39	0.97
1:C:110:PRO:CG	2:D:135:ASP:OD1	2.13	0.97
1:E:51:THR:CB	2:F:83:ARG:NH1	2.25	0.97
1:G:13:THR:HG21	2:H:5:ILE:HG21	1.47	0.97
1:E:13:THR:HG21	2:F:5:ILE:HG21	1.47	0.97
1:G:49:LEU:O	2:H:127:ALA:O	1.83	0.96
1:C:98:THR:N	2:F:449:LEU:CD2	2.27	0.96
2:B:16:SER:O	2:B:17:THR:HG23	1.65	0.96
2:F:142:LEU:HD12	2:F:146:LYS:HE3	0.98	0.96
2:H:16:SER:O	2:H:17:THR:HG23	1.65	0.96
2:F:16:SER:O	2:F:17:THR:HG23	1.65	0.96
2:H:142:LEU:HD12	2:H:146:LYS:HE3	0.98	0.96
2:H:142:LEU:HD11	2:H:146:LYS:HE3	1.42	0.95
1:E:98:THR:N	2:H:449:LEU:CD2	2.27	0.95
1:G:110:PRO:HB3	2:H:132:PRO:HD2	0.95	0.95
1:E:23:THR:HG23	2:H:95:VAL:CG2	1.96	0.95
1:G:77:ARG:HH21	2:H:16:SER:N	1.65	0.95
2:D:449:LEU:HD22	1:G:96:GLY:O	1.65	0.95
1:C:23:THR:CG2	2:F:95:VAL:CG2	2.44	0.95
1:E:98:THR:H	2:H:449:LEU:HD21	0.80	0.95
1:C:112:LEU:CD2	2:D:72:MET:HG3	1.97	0.95
2:D:16:SER:O	2:D:17:THR:HG23	1.65	0.94
1:A:77:ARG:HH21	2:B:16:SER:N	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HA	2:F:449:LEU:HD11	1.45	0.94
1:C:51:THR:HG23	2:D:83:ARG:HG2	1.44	0.94
1:G:51:THR:CG2	2:H:83:ARG:HH11	1.78	0.94
1:C:13:THR:HG21	2:D:5:ILE:HG21	1.47	0.94
1:C:23:THR:HG21	2:F:95:VAL:HB	1.47	0.94
1:G:112:LEU:CD2	2:H:76:LEU:HD21	1.97	0.94
1:E:77:ARG:HH21	2:F:16:SER:N	1.65	0.94
1:C:96:GLY:C	2:F:449:LEU:HD22	1.88	0.94
1:C:77:ARG:HH21	2:D:16:SER:N	1.65	0.94
1:G:51:THR:OG1	2:H:83:ARG:NH1	2.00	0.94
2:D:126:GLN:CA	2:D:131:VAL:CG2	2.47	0.93
1:C:51:THR:HB	2:D:83:ARG:NH1	1.71	0.93
2:F:132:PRO:HG2	2:F:135:ASP:HA	1.50	0.93
1:A:13:THR:HG21	2:B:5:ILE:HG21	1.47	0.93
1:E:49:LEU:HD13	2:F:367:GLU:CG	1.96	0.93
1:G:112:LEU:CD2	2:H:72:MET:HG3	1.98	0.93
1:C:112:LEU:HD23	2:D:72:MET:HG3	1.51	0.92
2:F:126:GLN:CA	2:F:131:VAL:CG2	2.47	0.92
2:D:131:VAL:HG13	2:D:132:PRO:HB3	1.43	0.92
2:B:132:PRO:HG2	2:B:135:ASP:HA	1.50	0.92
1:G:51:THR:CG2	2:H:83:ARG:HG3	1.99	0.92
1:E:26:GLN:HE22	1:E:60:ASP:H	1.17	0.92
2:H:132:PRO:HG2	2:H:135:ASP:HA	1.50	0.92
2:H:133:TRP:CZ3	2:H:142:LEU:HD23	2.05	0.92
1:G:49:LEU:HD13	2:H:367:GLU:HG3	1.51	0.92
1:A:26:GLN:HE22	1:A:60:ASP:H	1.17	0.92
1:G:79:SER:OG	2:H:9:HIS:ND1	2.02	0.92
2:B:131:VAL:CG1	2:B:132:PRO:HA	1.97	0.92
1:A:79:SER:OG	2:B:9:HIS:ND1	2.02	0.92
1:C:51:THR:CG2	2:D:83:ARG:HH11	1.83	0.92
2:D:133:TRP:CZ3	2:D:142:LEU:HD23	2.05	0.92
1:C:97:ILE:CA	2:F:449:LEU:HD21	2.00	0.92
1:C:112:LEU:CD1	2:D:76:LEU:HD22	2.00	0.91
2:F:115:LEU:HD23	2:F:144:ALA:HB1	1.51	0.91
2:D:115:LEU:HD23	2:D:144:ALA:HB1	1.51	0.91
2:H:126:GLN:CA	2:H:131:VAL:CG2	2.47	0.91
2:B:126:GLN:CA	2:B:131:VAL:CG2	2.47	0.91
2:B:133:TRP:CZ3	2:B:142:LEU:HD23	2.05	0.90
1:E:79:SER:OG	2:F:9:HIS:ND1	2.02	0.90
1:C:79:SER:OG	2:D:9:HIS:ND1	2.02	0.90
2:F:142:LEU:CD1	2:F:146:LYS:CE	2.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:LEU:HD23	2:H:144:ALA:HB1	1.51	0.90
2:H:131:VAL:CG1	2:H:132:PRO:HA	1.97	0.90
2:H:142:LEU:CD1	2:H:146:LYS:CE	2.32	0.90
1:G:112:LEU:CD1	2:H:76:LEU:CD2	2.50	0.90
2:B:115:LEU:HD23	2:B:144:ALA:HB1	1.51	0.90
2:B:257:GLY:HA2	1:G:257:THR:HG21	1.52	0.90
1:A:257:THR:HG21	2:H:257:GLY:HA2	1.53	0.90
2:D:131:VAL:CG1	2:D:132:PRO:HA	1.97	0.90
1:C:112:LEU:HD13	2:D:76:LEU:CD2	2.01	0.90
2:F:133:TRP:CZ3	2:F:142:LEU:HD23	2.05	0.90
2:D:132:PRO:HG2	2:D:135:ASP:HA	1.50	0.90
2:D:272:SER:C	1:G:6:ILE:HG13	1.92	0.90
1:A:77:ARG:HD3	2:B:136:LYS:HZ1	1.36	0.89
1:G:112:LEU:HD23	2:H:72:MET:HG3	1.52	0.89
1:A:51:THR:HB	2:B:83:ARG:HH11	1.36	0.89
1:G:26:GLN:HE22	1:G:60:ASP:H	1.17	0.89
2:F:131:VAL:CG1	2:F:132:PRO:HA	1.96	0.89
1:C:26:GLN:HE22	1:C:60:ASP:H	1.17	0.89
1:E:79:SER:HB2	2:F:9:HIS:HB3	1.54	0.88
1:G:79:SER:HB2	2:H:9:HIS:HB3	1.54	0.88
1:A:79:SER:HB2	2:B:9:HIS:HB3	1.54	0.88
1:E:49:LEU:CD1	2:F:367:GLU:HG3	2.01	0.88
1:C:110:PRO:HG3	2:D:135:ASP:CG	1.93	0.88
1:G:51:THR:CG2	2:H:83:ARG:CD	2.51	0.88
1:G:112:LEU:HD13	2:H:76:LEU:CD2	2.04	0.87
1:E:219:ASP:OD1	2:F:11:VAL:HG22	1.74	0.87
1:C:294:HIS:CE1	2:D:7:PRO:HG3	2.09	0.87
1:G:294:HIS:CE1	2:H:7:PRO:HG3	2.10	0.87
1:E:23:THR:HG21	2:H:95:VAL:CG2	2.03	0.87
1:C:77:ARG:NH2	2:D:15:GLU:HB3	1.90	0.87
1:A:77:ARG:NH2	2:B:15:GLU:HB3	1.90	0.87
1:C:98:THR:H	2:F:449:LEU:HD21	1.35	0.86
1:A:219:ASP:OD1	2:B:11:VAL:HG22	1.75	0.86
1:E:294:HIS:CE1	2:F:7:PRO:HG3	2.10	0.86
2:F:126:GLN:O	2:F:131:VAL:CB	2.23	0.86
1:C:97:ILE:HA	2:F:449:LEU:CD2	2.05	0.86
1:G:112:LEU:CD1	2:H:76:LEU:HD22	2.04	0.86
1:G:112:LEU:HD11	2:H:76:LEU:HD22	1.54	0.86
1:C:219:ASP:OD1	2:D:11:VAL:HG22	1.75	0.86
1:E:224:TYR:CE2	1:E:294:HIS:NE2	2.44	0.86
1:G:224:TYR:CE2	1:G:294:HIS:NE2	2.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:ASP:OD1	2:H:11:VAL:HG22	1.75	0.86
2:B:126:GLN:O	2:B:131:VAL:CB	2.23	0.86
1:A:294:HIS:CE1	2:B:7:PRO:HG3	2.10	0.86
2:H:126:GLN:O	2:H:131:VAL:CB	2.23	0.86
1:A:224:TYR:CE2	1:A:294:HIS:NE2	2.44	0.86
1:G:77:ARG:NH2	2:H:15:GLU:HB3	1.90	0.86
1:C:79:SER:HB2	2:D:9:HIS:HB3	1.55	0.85
1:G:51:THR:HG1	2:H:83:ARG:HD3	1.36	0.85
1:A:51:THR:CG2	2:B:83:ARG:HG3	1.92	0.85
1:C:97:ILE:CA	2:F:449:LEU:CD2	2.53	0.85
1:C:224:TYR:CE2	1:C:294:HIS:NE2	2.44	0.85
1:E:158:ASN:ND2	1:E:159:ARG:H	1.75	0.85
2:D:126:GLN:O	2:D:131:VAL:CB	2.23	0.85
1:G:112:LEU:CD2	2:H:76:LEU:CD2	2.53	0.85
1:E:77:ARG:NH2	2:F:15:GLU:HB3	1.90	0.85
2:F:132:PRO:CG	2:F:135:ASP:HA	2.07	0.85
2:B:132:PRO:CG	2:B:135:ASP:HA	2.07	0.85
1:E:112:LEU:CD2	2:F:76:LEU:CD2	2.54	0.85
2:H:132:PRO:CG	2:H:135:ASP:HA	2.07	0.85
1:G:51:THR:HB	2:H:83:ARG:NH1	1.90	0.85
1:C:112:LEU:HD22	2:D:76:LEU:CD2	2.07	0.85
1:G:49:LEU:HB3	2:H:127:ALA:HB3	1.58	0.85
1:E:51:THR:HB	2:F:83:ARG:NH1	1.87	0.84
2:D:132:PRO:HG2	2:D:135:ASP:N	1.91	0.84
2:D:95:VAL:HG21	1:G:23:THR:CG2	2.06	0.84
1:A:158:ASN:ND2	1:A:159:ARG:H	1.75	0.84
1:C:110:PRO:HG3	2:D:135:ASP:OD1	1.74	0.84
2:D:3:VAL:HA	2:D:4:TYR:HB3	1.60	0.84
2:D:3:VAL:HA	2:D:4:TYR:CB	2.07	0.84
2:D:285:THR:HG22	2:D:343:THR:HG22	1.60	0.84
1:G:110:PRO:HG3	2:H:135:ASP:CG	1.97	0.84
2:F:3:VAL:HA	2:F:4:TYR:HB3	1.60	0.84
2:D:132:PRO:CG	2:D:135:ASP:HA	2.07	0.84
2:B:132:PRO:HG2	2:B:135:ASP:N	1.91	0.84
2:D:142:LEU:CD1	2:D:146:LYS:CE	2.32	0.84
2:H:132:PRO:HG2	2:H:135:ASP:N	1.91	0.84
1:G:158:ASN:ND2	1:G:159:ARG:H	1.75	0.83
1:C:158:ASN:ND2	1:C:159:ARG:H	1.75	0.83
2:B:285:THR:HG22	2:B:343:THR:HG22	1.60	0.83
2:F:132:PRO:HG2	2:F:135:ASP:N	1.91	0.83
1:E:51:THR:OG1	2:F:83:ARG:NH1	2.02	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:VAL:HA	2:F:4:TYR:CB	2.07	0.83
2:H:285:THR:HG22	2:H:343:THR:HG22	1.60	0.83
2:H:3:VAL:HA	2:H:4:TYR:CB	2.07	0.82
2:F:285:THR:HG22	2:F:343:THR:HG22	1.60	0.82
1:C:97:ILE:C	2:F:449:LEU:CD2	2.47	0.82
2:B:3:VAL:HA	2:B:4:TYR:CB	2.07	0.82
1:C:149:LYS:HA	1:C:149:LYS:HE3	1.61	0.82
2:F:131:VAL:HG13	2:F:132:PRO:HB3	1.43	0.81
1:E:149:LYS:HA	1:E:149:LYS:HE3	1.61	0.81
1:A:77:ARG:HD3	2:B:136:LYS:NZ	1.94	0.81
2:H:3:VAL:HA	2:H:4:TYR:HB3	1.60	0.81
1:E:112:LEU:CD2	2:F:76:LEU:HD21	2.10	0.81
1:G:51:THR:HB	2:H:83:ARG:HH11	1.40	0.81
2:B:3:VAL:HA	2:B:4:TYR:HB3	1.60	0.81
1:A:80:THR:HG23	2:B:9:HIS:HB3	1.63	0.81
1:E:158:ASN:HD22	1:E:159:ARG:H	1.27	0.81
2:H:115:LEU:CD2	2:H:144:ALA:HB1	2.11	0.81
1:G:149:LYS:HE3	1:G:149:LYS:HA	1.61	0.81
2:D:115:LEU:CD2	2:D:144:ALA:HB1	2.11	0.81
1:C:80:THR:HG23	2:D:9:HIS:HB3	1.63	0.81
1:A:51:THR:CB	2:B:83:ARG:NH1	2.43	0.81
2:F:126:GLN:C	2:F:131:VAL:CG2	2.49	0.80
2:B:115:LEU:CD2	2:B:144:ALA:HB1	2.11	0.80
1:G:224:TYR:CD2	1:G:294:HIS:CD2	2.69	0.80
2:F:115:LEU:CD2	2:F:144:ALA:HB1	2.11	0.80
1:C:224:TYR:CD2	1:C:294:HIS:CD2	2.69	0.80
1:G:79:SER:CB	2:H:9:HIS:ND1	2.45	0.80
2:B:126:GLN:C	2:B:131:VAL:CG2	2.49	0.80
1:A:79:SER:CB	2:B:9:HIS:ND1	2.45	0.80
1:E:224:TYR:CD2	1:E:294:HIS:CD2	2.69	0.80
1:A:149:LYS:HE3	1:A:149:LYS:HA	1.61	0.80
2:H:126:GLN:C	2:H:131:VAL:CG2	2.49	0.80
2:B:126:GLN:CB	2:B:131:VAL:HG21	2.12	0.80
1:E:79:SER:CB	2:F:9:HIS:ND1	2.45	0.80
2:D:126:GLN:C	2:D:131:VAL:CG2	2.49	0.80
1:C:79:SER:CB	2:D:9:HIS:ND1	2.45	0.80
2:H:126:GLN:CB	2:H:131:VAL:HG21	2.12	0.80
1:G:49:LEU:HB3	2:H:127:ALA:CB	2.12	0.80
1:E:80:THR:HG23	2:F:9:HIS:HB3	1.63	0.80
2:F:126:GLN:CB	2:F:131:VAL:HG21	2.12	0.80
1:G:112:LEU:HD22	2:H:76:LEU:CD2	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:LEU:CD2	1:G:98:THR:N	2.42	0.79
2:B:142:LEU:CD1	2:B:146:LYS:CE	2.32	0.79
1:G:80:THR:HG23	2:H:9:HIS:HB3	1.63	0.79
1:A:9:ASN:HD21	1:A:12:ASP:H	1.30	0.79
1:C:158:ASN:HD22	1:C:159:ARG:H	1.28	0.79
1:C:112:LEU:CD1	2:D:76:LEU:CD2	2.59	0.79
1:C:23:THR:CG2	2:F:95:VAL:HB	2.12	0.79
1:A:224:TYR:CD2	1:A:294:HIS:CD2	2.69	0.79
2:D:126:GLN:O	2:D:131:VAL:HB	1.83	0.79
1:A:77:ARG:HD2	2:B:15:GLU:HA	1.66	0.78
1:C:9:ASN:HD21	1:C:12:ASP:H	1.30	0.78
2:D:126:GLN:CB	2:D:131:VAL:HG21	2.12	0.78
1:E:274:SER:O	1:E:278:VAL:HG13	1.84	0.78
1:E:9:ASN:HD21	1:E:12:ASP:H	1.30	0.78
1:A:158:ASN:HD22	1:A:159:ARG:H	1.28	0.78
1:A:274:SER:O	1:A:278:VAL:HG13	1.84	0.78
1:G:77:ARG:NH2	2:H:16:SER:N	2.32	0.78
2:F:126:GLN:O	2:F:131:VAL:HB	1.84	0.78
1:G:112:LEU:HD13	2:H:76:LEU:HD21	1.65	0.78
1:G:158:ASN:HD22	1:G:159:ARG:H	1.27	0.78
2:B:126:GLN:O	2:B:131:VAL:HB	1.84	0.77
1:G:274:SER:O	1:G:278:VAL:HG13	1.84	0.77
1:C:77:ARG:NH2	2:D:16:SER:N	2.32	0.77
2:D:5:ILE:HG22	2:D:6:HIS:N	2.00	0.77
1:E:13:THR:CG2	2:F:5:ILE:HG21	2.15	0.77
1:G:224:TYR:CD2	1:G:294:HIS:NE2	2.53	0.77
1:C:274:SER:O	1:C:278:VAL:HG13	1.84	0.77
1:E:224:TYR:CD2	1:E:294:HIS:NE2	2.53	0.76
1:E:96:GLY:O	2:H:447:ASN:ND2	2.18	0.76
1:C:13:THR:CG2	2:D:5:ILE:HG21	2.15	0.76
1:G:49:LEU:CB	2:H:127:ALA:HB3	2.16	0.76
1:G:77:ARG:HD2	2:H:15:GLU:HA	1.65	0.76
1:A:77:ARG:NH2	2:B:16:SER:N	2.32	0.76
1:A:49:LEU:O	2:B:127:ALA:O	2.03	0.76
1:C:112:LEU:HD11	2:D:76:LEU:HD22	1.68	0.76
2:H:5:ILE:HG22	2:H:6:HIS:N	2.00	0.76
1:C:112:LEU:CD2	2:D:76:LEU:CD2	2.63	0.76
1:G:9:ASN:HD21	1:G:12:ASP:H	1.30	0.76
1:C:110:PRO:HB2	2:D:135:ASP:OD1	1.84	0.76
2:H:126:GLN:O	2:H:131:VAL:HB	1.84	0.76
1:E:77:ARG:NH2	2:F:16:SER:N	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:CD2	1:C:294:HIS:NE2	2.53	0.76
2:B:320:LEU:HD11	2:B:426:PRO:HB2	1.68	0.76
2:H:320:LEU:HD11	2:H:426:PRO:HB2	1.68	0.76
2:F:320:LEU:HD11	2:F:426:PRO:HB2	1.68	0.76
2:F:5:ILE:HG22	2:F:6:HIS:N	2.00	0.76
1:E:49:LEU:O	2:F:127:ALA:O	2.03	0.76
1:A:224:TYR:CD2	1:A:294:HIS:NE2	2.53	0.76
1:A:51:THR:HB	2:B:83:ARG:NH1	2.01	0.76
1:C:77:ARG:HD2	2:D:15:GLU:HA	1.66	0.75
1:E:77:ARG:HD2	2:F:15:GLU:HA	1.66	0.75
1:A:13:THR:CG2	2:B:5:ILE:HG21	2.15	0.75
2:D:320:LEU:HD11	2:D:426:PRO:HB2	1.68	0.75
1:G:13:THR:CG2	2:H:5:ILE:HG21	2.15	0.75
2:D:142:LEU:O	2:D:146:LYS:HB2	1.87	0.75
1:G:51:THR:HG21	2:H:83:ARG:HH11	1.49	0.75
1:A:296:MET:HG2	2:B:9:HIS:NE2	2.02	0.75
1:E:96:GLY:O	2:H:449:LEU:HD22	1.87	0.74
1:E:296:MET:HG2	2:F:9:HIS:NE2	2.02	0.74
1:A:245:LEU:CD1	2:B:68:LEU:CD2	2.26	0.74
1:A:110:PRO:CB	2:B:132:PRO:HD2	2.07	0.74
1:C:296:MET:HG2	2:D:9:HIS:NE2	2.02	0.74
2:H:3:VAL:O	2:H:3:VAL:HG23	1.88	0.74
1:G:51:THR:HG23	2:H:83:ARG:CD	2.16	0.74
2:B:5:ILE:HG22	2:B:6:HIS:N	2.00	0.74
2:F:5:ILE:HG22	2:F:6:HIS:H	1.53	0.74
1:G:296:MET:HG2	2:H:9:HIS:NE2	2.02	0.74
2:F:142:LEU:O	2:F:146:LYS:HB2	1.87	0.73
2:F:3:VAL:HG23	2:F:3:VAL:O	1.88	0.73
1:A:77:ARG:HH21	2:B:16:SER:H	1.36	0.73
2:D:3:VAL:CB	2:D:4:TYR:CD2	2.62	0.73
2:D:5:ILE:HG22	2:D:6:HIS:H	1.53	0.73
1:G:80:THR:HG23	2:H:9:HIS:CB	2.19	0.73
1:E:112:LEU:CD1	2:F:76:LEU:HD22	2.19	0.73
2:B:176:VAL:HG23	2:B:198:THR:HG21	1.71	0.73
2:D:161:GLN:CB	2:D:168:ALA:HB2	2.19	0.73
2:F:161:GLN:CB	2:F:168:ALA:HB2	2.18	0.73
2:H:123:ASP:HA	2:H:126:GLN:OE1	1.89	0.73
1:G:51:THR:HG23	2:H:83:ARG:HG2	1.67	0.73
1:E:77:ARG:HH21	2:F:16:SER:H	1.36	0.73
1:A:80:THR:HG23	2:B:9:HIS:CB	2.19	0.73
2:F:123:ASP:HA	2:F:126:GLN:OE1	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:LEU:O	2:H:146:LYS:HB2	1.87	0.72
2:B:142:LEU:O	2:B:146:LYS:HB2	1.87	0.72
2:B:123:ASP:HA	2:B:126:GLN:OE1	1.89	0.72
1:E:110:PRO:CB	2:F:135:ASP:OD1	2.37	0.72
2:B:3:VAL:O	2:B:3:VAL:HG23	1.88	0.72
2:H:5:ILE:HG22	2:H:6:HIS:H	1.53	0.72
2:F:132:PRO:HG2	2:F:135:ASP:H	1.54	0.72
1:G:51:THR:HG23	2:H:83:ARG:HD3	1.70	0.72
1:C:80:THR:HG23	2:D:9:HIS:CB	2.19	0.72
1:C:49:LEU:HB3	2:D:127:ALA:CB	2.20	0.72
1:E:80:THR:HG23	2:F:9:HIS:CB	2.19	0.72
2:D:176:VAL:HG23	2:D:198:THR:HG21	1.71	0.72
2:F:16:SER:O	2:F:17:THR:CG2	2.37	0.72
2:F:176:VAL:HG23	2:F:198:THR:HG21	1.71	0.72
2:H:69:ARG:HG3	2:H:133:TRP:HZ2	1.55	0.72
1:C:23:THR:CG2	2:F:95:VAL:CB	2.68	0.72
1:G:112:LEU:CD1	2:H:76:LEU:HD21	2.18	0.72
2:B:143:ASP:O	2:B:144:ALA:HB3	1.89	0.72
2:B:161:GLN:CB	2:B:168:ALA:HB2	2.19	0.72
2:H:132:PRO:HG2	2:H:135:ASP:H	1.54	0.71
2:H:176:VAL:HG23	2:H:198:THR:HG21	1.71	0.71
2:D:69:ARG:HG3	2:D:133:TRP:HZ2	1.55	0.71
2:H:161:GLN:CB	2:H:168:ALA:HB2	2.19	0.71
1:E:77:ARG:HD3	2:F:136:LYS:HZ1	1.54	0.71
2:D:3:VAL:O	2:D:3:VAL:HG23	1.88	0.71
2:B:3:VAL:CB	2:B:4:TYR:CD2	2.63	0.71
1:E:70:ASN:HB2	1:E:102:MET:HE1	1.73	0.71
1:C:77:ARG:HH21	2:D:16:SER:H	1.36	0.71
2:D:123:ASP:HA	2:D:126:GLN:OE1	1.89	0.71
1:C:77:ARG:HD3	2:D:136:LYS:HZ1	1.56	0.71
2:F:69:ARG:HG3	2:F:133:TRP:HZ2	1.55	0.71
2:D:142:LEU:HD12	2:D:146:LYS:HE2	1.70	0.71
2:H:143:ASP:O	2:H:144:ALA:HB3	1.89	0.71
2:F:142:LEU:HD12	2:F:146:LYS:HE2	1.70	0.71
2:B:285:THR:HG23	1:G:283:TYR:HB2	1.73	0.71
2:B:5:ILE:HG22	2:B:6:HIS:H	1.53	0.71
2:B:69:ARG:HG3	2:B:133:TRP:HZ2	1.55	0.71
2:B:16:SER:O	2:B:17:THR:CG2	2.37	0.71
2:H:16:SER:O	2:H:17:THR:CG2	2.37	0.70
1:G:49:LEU:C	2:H:127:ALA:HB1	2.11	0.70
1:A:49:LEU:HD13	2:B:367:GLU:CG	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:LEU:HD11	2:F:379:GLN:CG	2.22	0.70
2:D:118:LEU:HD11	2:D:379:GLN:CG	2.21	0.70
2:F:3:VAL:CB	2:F:4:TYR:CD2	2.63	0.70
2:D:95:VAL:CG2	1:G:23:THR:CG2	2.68	0.70
1:C:49:LEU:HD13	2:D:367:GLU:CG	2.13	0.70
2:F:143:ASP:O	2:F:144:ALA:HB3	1.89	0.70
1:G:244:ARG:HD3	1:G:247:ASP:OD2	1.92	0.70
1:A:77:ARG:CD	2:B:136:LYS:HZ1	2.05	0.70
2:H:118:LEU:HD11	2:H:379:GLN:CG	2.21	0.70
2:B:118:LEU:HD11	2:B:379:GLN:CG	2.21	0.70
2:B:132:PRO:HG2	2:B:135:ASP:H	1.54	0.70
1:E:244:ARG:HD3	1:E:247:ASP:OD2	1.92	0.70
2:B:142:LEU:HD12	2:B:146:LYS:HE2	1.70	0.70
2:D:143:ASP:O	2:D:144:ALA:HB3	1.89	0.70
1:G:77:ARG:HH21	2:H:16:SER:H	1.36	0.70
1:G:51:THR:HG21	2:H:83:ARG:CG	2.12	0.70
1:A:110:PRO:CB	2:B:135:ASP:OD1	2.40	0.69
2:H:3:VAL:CB	2:H:4:TYR:CD2	2.62	0.69
2:B:132:PRO:O	2:B:134:LYS:N	2.24	0.69
1:C:244:ARG:HD3	1:C:247:ASP:OD2	1.92	0.69
1:G:70:ASN:HB2	1:G:102:MET:HE1	1.75	0.69
1:A:70:ASN:HB2	1:A:102:MET:HE1	1.75	0.69
2:D:16:SER:O	2:D:17:THR:CG2	2.37	0.69
1:C:97:ILE:HA	2:F:449:LEU:HD13	1.74	0.69
1:G:112:LEU:CD2	2:H:72:MET:CG	2.71	0.69
2:D:329:GLN:N	2:D:333:LEU:HD21	2.08	0.69
1:G:296:MET:HG2	2:H:9:HIS:CE1	2.28	0.69
1:A:296:MET:HG2	2:B:9:HIS:CE1	2.28	0.69
1:E:9:ASN:C	1:E:9:ASN:HD22	1.96	0.69
2:F:329:GLN:N	2:F:333:LEU:HD21	2.08	0.69
1:A:244:ARG:HD3	1:A:247:ASP:OD2	1.92	0.69
2:B:329:GLN:N	2:B:333:LEU:HD21	2.08	0.69
2:D:132:PRO:HG2	2:D:135:ASP:H	1.54	0.69
2:B:135:ASP:O	2:B:136:LYS:HG3	1.93	0.69
1:C:70:ASN:HB2	1:C:102:MET:HE1	1.74	0.69
1:G:82:THR:OG1	2:H:136:LYS:HE3	1.93	0.68
2:H:135:ASP:O	2:H:136:LYS:HG3	1.93	0.68
1:A:77:ARG:HD2	2:B:15:GLU:HG2	1.75	0.68
2:H:132:PRO:CG	2:H:135:ASP:CA	2.68	0.68
2:B:69:ARG:NH1	2:B:133:TRP:CH2	2.62	0.68
1:E:77:ARG:HD2	2:F:15:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:ARG:NH1	2:H:133:TRP:CH2	2.62	0.68
1:G:110:PRO:HG3	2:H:135:ASP:OD1	1.88	0.68
1:G:9:ASN:HD22	1:G:9:ASN:C	1.96	0.68
2:D:135:ASP:O	2:D:136:LYS:HG3	1.93	0.68
2:F:132:PRO:O	2:F:134:LYS:N	2.24	0.68
2:F:69:ARG:NH1	2:F:133:TRP:CH2	2.62	0.68
1:E:296:MET:HG2	2:F:9:HIS:CE1	2.28	0.68
1:C:296:MET:HG2	2:D:9:HIS:CE1	2.28	0.68
1:A:9:ASN:C	1:A:9:ASN:HD22	1.96	0.68
2:B:134:LYS:O	2:B:135:ASP:HB2	1.93	0.68
1:A:224:TYR:CE2	2:B:7:PRO:HB3	2.29	0.68
2:D:69:ARG:NH1	2:D:133:TRP:CH2	2.62	0.68
1:C:77:ARG:HD2	2:D:15:GLU:HG2	1.75	0.68
2:H:132:PRO:O	2:H:134:LYS:N	2.24	0.68
1:A:77:ARG:CD	2:B:136:LYS:NZ	2.57	0.68
1:G:79:SER:HB2	2:H:9:HIS:CB	2.24	0.68
1:C:79:SER:HB2	2:D:9:HIS:CB	2.24	0.68
2:H:329:GLN:N	2:H:333:LEU:HD21	2.08	0.68
1:C:23:THR:CG2	2:F:95:VAL:HG21	2.06	0.67
1:A:257:THR:OG1	2:H:403:GLU:O	2.09	0.67
1:C:224:TYR:CE2	2:D:7:PRO:HB3	2.29	0.67
2:H:134:LYS:O	2:H:135:ASP:HB2	1.93	0.67
2:F:134:LYS:O	2:F:135:ASP:HB2	1.93	0.67
2:D:134:LYS:O	2:D:135:ASP:HB2	1.93	0.67
1:C:49:LEU:CB	2:D:127:ALA:HB3	2.25	0.67
1:E:79:SER:HB2	2:F:9:HIS:CB	2.24	0.67
1:G:224:TYR:CE2	2:H:7:PRO:HB3	2.29	0.67
1:C:112:LEU:CD2	2:D:76:LEU:HD21	2.18	0.67
1:C:112:LEU:HD13	2:D:76:LEU:HD21	1.74	0.67
1:G:49:LEU:CB	2:H:127:ALA:CB	2.73	0.67
1:G:77:ARG:HD2	2:H:15:GLU:HG2	1.75	0.67
1:E:110:PRO:CG	2:F:135:ASP:OD1	2.43	0.67
1:C:9:ASN:HD22	1:C:9:ASN:C	1.96	0.67
2:B:84:ILE:HG21	2:B:362:LEU:HD11	1.77	0.67
1:A:110:PRO:CG	2:B:135:ASP:OD1	2.42	0.67
1:E:224:TYR:CE2	2:F:7:PRO:HB3	2.29	0.67
2:F:135:ASP:O	2:F:136:LYS:HG3	1.93	0.67
1:A:112:LEU:CD1	2:B:76:LEU:HD22	2.24	0.67
2:H:84:ILE:HG21	2:H:362:LEU:HD11	1.77	0.67
2:H:141:ARG:O	2:H:146:LYS:HG2	1.90	0.66
1:C:77:ARG:CD	2:D:136:LYS:HZ1	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:PRO:CG	2:H:135:ASP:CG	2.59	0.66
1:A:36:SER:HA	2:B:12:ILE:CG2	2.25	0.66
1:A:9:ASN:HD22	1:A:10:TYR:N	1.93	0.66
2:B:118:LEU:HD11	2:B:379:GLN:CD	2.16	0.66
2:F:106:VAL:HG13	2:F:359:LEU:HD11	1.77	0.66
1:G:36:SER:HA	2:H:12:ILE:CG2	2.25	0.66
1:G:9:ASN:HD22	1:G:10:TYR:N	1.93	0.66
2:F:84:ILE:HG21	2:F:362:LEU:HD11	1.77	0.66
2:D:14:ASN:N	2:D:14:ASN:HD22	1.94	0.66
2:D:118:LEU:HD11	2:D:379:GLN:CD	2.16	0.66
1:E:229:THR:O	1:E:233:GLU:HG2	1.96	0.66
1:C:49:LEU:HB3	2:D:127:ALA:HB3	1.76	0.66
1:A:79:SER:HB2	2:B:9:HIS:CB	2.24	0.66
1:C:229:THR:O	1:C:233:GLU:HG2	1.96	0.66
1:E:9:ASN:HD22	1:E:10:TYR:N	1.93	0.66
2:D:84:ILE:HG21	2:D:362:LEU:HD11	1.77	0.66
2:H:3:VAL:HB	2:H:4:TYR:CE2	2.30	0.66
2:H:118:LEU:HD11	2:H:379:GLN:CD	2.16	0.66
2:H:14:ASN:N	2:H:14:ASN:HD22	1.94	0.66
2:F:128:ILE:HG23	2:F:367:GLU:HG2	1.78	0.66
1:C:110:PRO:HB3	2:D:132:PRO:CD	2.16	0.65
2:D:3:VAL:O	2:D:3:VAL:CG2	2.44	0.65
2:F:3:VAL:HB	2:F:4:TYR:CE2	2.30	0.65
1:A:112:LEU:HD13	2:B:76:LEU:CD1	2.26	0.65
2:D:132:PRO:O	2:D:134:LYS:N	2.24	0.65
2:F:14:ASN:HD22	2:F:14:ASN:N	1.94	0.65
1:G:229:THR:O	1:G:233:GLU:HG2	1.96	0.65
1:A:229:THR:O	1:A:233:GLU:HG2	1.96	0.65
2:B:3:VAL:HB	2:B:4:TYR:CE2	2.31	0.65
2:H:3:VAL:CG2	2:H:3:VAL:O	2.44	0.65
1:C:36:SER:HA	2:D:12:ILE:CG2	2.25	0.65
2:F:118:LEU:HD11	2:F:379:GLN:CD	2.16	0.65
2:B:4:TYR:CD1	2:B:5:ILE:HD12	2.32	0.65
2:B:128:ILE:HG23	2:B:367:GLU:HG2	1.78	0.65
2:D:3:VAL:HB	2:D:4:TYR:CE2	2.30	0.65
1:A:245:LEU:H	2:B:68:LEU:HD21	1.60	0.65
2:D:106:VAL:HG13	2:D:359:LEU:HD11	1.77	0.65
2:B:106:VAL:HG13	2:B:359:LEU:HD11	1.77	0.65
2:H:249:VAL:CG1	2:H:395:ILE:HG22	2.27	0.65
2:B:249:VAL:CG1	2:B:395:ILE:HG22	2.27	0.65
2:B:14:ASN:N	2:B:14:ASN:HD22	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:HG21	2:F:95:VAL:CB	2.25	0.65
2:D:128:ILE:HG23	2:D:367:GLU:HG2	1.78	0.65
1:G:49:LEU:O	2:H:127:ALA:C	2.33	0.65
2:H:128:ILE:HG23	2:H:367:GLU:HG2	1.78	0.65
2:H:106:VAL:HG13	2:H:359:LEU:HD11	1.77	0.65
1:E:36:SER:HA	2:F:12:ILE:CG2	2.25	0.65
1:E:112:LEU:HD13	2:F:76:LEU:CD2	2.26	0.65
1:C:9:ASN:HD22	1:C:10:TYR:N	1.93	0.65
1:A:208:LEU:HD12	1:A:209:LEU:HG	1.79	0.65
2:H:4:TYR:CD1	2:H:5:ILE:HD12	2.32	0.65
1:E:110:PRO:HG3	2:F:135:ASP:OD1	1.97	0.65
2:D:4:TYR:CD1	2:D:5:ILE:HD12	2.32	0.65
2:B:3:VAL:CG2	2:B:3:VAL:O	2.44	0.65
1:C:208:LEU:HD12	1:C:209:LEU:HG	1.79	0.65
2:F:3:VAL:CG2	2:F:3:VAL:O	2.44	0.64
1:C:49:LEU:CB	2:D:127:ALA:CB	2.75	0.64
2:B:144:ALA:O	2:B:148:LEU:HG	1.97	0.64
2:D:249:VAL:CG1	2:D:395:ILE:HG22	2.27	0.64
1:C:6:ILE:CG1	2:F:272:SER:O	2.44	0.64
1:C:273:THR:HG22	1:C:275:ALA:H	1.63	0.64
1:E:208:LEU:HD12	1:E:209:LEU:HG	1.79	0.64
2:H:142:LEU:HD12	2:H:146:LYS:HE2	1.70	0.64
1:A:273:THR:HG22	1:A:275:ALA:H	1.63	0.64
2:F:249:VAL:CG1	2:F:395:ILE:HG22	2.27	0.64
1:C:36:SER:HA	2:D:12:ILE:HG21	1.80	0.64
2:B:142:LEU:HD12	2:B:146:LYS:CD	2.27	0.64
2:F:133:TRP:CH2	2:F:142:LEU:HD23	2.33	0.64
1:E:273:THR:HG22	1:E:275:ALA:H	1.63	0.64
2:B:133:TRP:CH2	2:B:142:LEU:HD23	2.33	0.64
2:F:4:TYR:CD1	2:F:5:ILE:HD12	2.32	0.64
1:E:219:ASP:OD1	2:F:11:VAL:CG2	2.45	0.64
1:G:273:THR:HG22	1:G:275:ALA:H	1.63	0.64
2:H:144:ALA:O	2:H:148:LEU:HG	1.97	0.63
2:F:142:LEU:HD12	2:F:146:LYS:CD	2.27	0.63
1:C:96:GLY:HA2	2:F:447:ASN:ND2	2.14	0.63
2:F:144:ALA:O	2:F:148:LEU:HG	1.97	0.63
1:A:36:SER:HA	2:B:12:ILE:HG21	1.80	0.63
1:G:219:ASP:OD1	2:H:11:VAL:CG2	2.46	0.63
1:C:23:THR:HG23	2:F:95:VAL:CB	2.29	0.63
2:D:144:ALA:O	2:D:148:LEU:HG	1.97	0.63
2:D:133:TRP:CH2	2:D:142:LEU:HD23	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:SER:HA	2:F:12:ILE:HG21	1.80	0.63
1:G:208:LEU:HD12	1:G:209:LEU:HG	1.79	0.63
1:G:77:ARG:NE	2:H:136:LYS:HZ3	1.96	0.63
2:H:133:TRP:CH2	2:H:142:LEU:HD23	2.33	0.63
1:C:219:ASP:OD1	2:D:11:VAL:CG2	2.46	0.63
2:F:131:VAL:CG1	2:F:132:PRO:N	2.58	0.63
1:G:36:SER:HA	2:H:12:ILE:HG21	1.80	0.62
1:E:112:LEU:HD23	2:F:72:MET:HG3	1.81	0.62
1:A:158:ASN:ND2	1:A:159:ARG:N	2.47	0.62
1:A:112:LEU:HD21	2:B:76:LEU:CD2	2.30	0.62
1:G:77:ARG:HD3	2:H:136:LYS:NZ	2.14	0.62
1:E:158:ASN:ND2	1:E:159:ARG:N	2.47	0.62
1:A:219:ASP:OD1	2:B:11:VAL:CG2	2.46	0.62
1:A:158:ASN:HD22	1:A:159:ARG:N	1.97	0.62
2:H:131:VAL:CG1	2:H:132:PRO:N	2.58	0.62
2:F:142:LEU:HD12	2:F:146:LYS:CG	2.30	0.62
1:G:158:ASN:HD22	1:G:159:ARG:N	1.97	0.62
1:G:158:ASN:ND2	1:G:159:ARG:N	2.47	0.62
2:B:118:LEU:HD21	2:B:379:GLN:HG3	1.82	0.62
2:F:131:VAL:HG12	2:F:132:PRO:CD	2.30	0.62
1:G:51:THR:HG1	2:H:83:ARG:CD	1.96	0.62
1:E:13:THR:CG2	2:F:5:ILE:CG2	2.72	0.61
1:E:158:ASN:HD22	1:E:159:ARG:N	1.97	0.61
2:D:118:LEU:HD21	2:D:379:GLN:HG3	1.82	0.61
1:C:77:ARG:CD	2:D:15:GLU:HG2	2.31	0.61
2:D:131:VAL:HG12	2:D:132:PRO:CD	2.30	0.61
1:G:99:VAL:HG12	1:G:145:GLN:OE1	2.01	0.61
1:A:77:ARG:CD	2:B:15:GLU:HG2	2.31	0.61
1:E:77:ARG:CZ	2:F:15:GLU:HB3	2.30	0.61
1:E:23:THR:CG2	2:H:95:VAL:HG23	2.27	0.61
1:C:6:ILE:HG13	2:F:272:SER:C	2.20	0.61
1:G:217:LEU:HD13	1:G:219:ASP:HB2	1.83	0.61
1:C:9:ASN:HD21	1:C:12:ASP:N	1.99	0.61
1:E:99:VAL:HG12	1:E:145:GLN:OE1	2.01	0.61
1:C:77:ARG:CZ	2:D:15:GLU:HB3	2.30	0.61
1:G:77:ARG:CD	2:H:15:GLU:HG2	2.31	0.61
2:H:131:VAL:HG12	2:H:132:PRO:CD	2.30	0.61
1:A:257:THR:CB	2:H:403:GLU:O	2.47	0.61
2:D:142:LEU:HD12	2:D:146:LYS:CG	2.30	0.61
1:G:77:ARG:NH2	2:H:16:SER:O	2.34	0.61
2:H:142:LEU:HD12	2:H:146:LYS:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:NH2	2:B:16:SER:O	2.34	0.61
1:C:296:MET:HG2	2:D:9:HIS:CD2	2.36	0.61
2:B:403:GLU:O	1:G:257:THR:HB	2.01	0.61
1:C:158:ASN:ND2	1:C:159:ARG:N	2.47	0.61
1:G:77:ARG:CZ	2:H:15:GLU:HB3	2.30	0.60
2:B:142:LEU:CD1	2:B:146:LYS:CG	2.77	0.60
2:F:132:PRO:CG	2:F:135:ASP:CA	2.67	0.60
1:A:51:THR:OG1	2:B:83:ARG:NH1	2.28	0.60
1:A:296:MET:HG2	2:B:9:HIS:CD2	2.36	0.60
2:H:142:LEU:HD12	2:H:146:LYS:CD	2.28	0.60
1:E:77:ARG:NH2	2:F:16:SER:O	2.34	0.60
1:C:217:LEU:HD13	1:C:219:ASP:HB2	1.83	0.60
2:F:118:LEU:HD21	2:F:379:GLN:HG3	1.82	0.60
2:H:118:LEU:HD21	2:H:379:GLN:HG3	1.82	0.60
2:B:131:VAL:CG1	2:B:132:PRO:N	2.58	0.60
1:G:112:LEU:HD13	2:H:76:LEU:CD1	2.30	0.60
1:A:217:LEU:HD13	1:A:219:ASP:HB2	1.83	0.60
1:E:296:MET:HG2	2:F:9:HIS:CD2	2.36	0.60
1:E:9:ASN:HD21	1:E:12:ASP:N	1.99	0.60
1:A:99:VAL:HG12	1:A:145:GLN:OE1	2.01	0.60
1:C:99:VAL:HG12	1:C:145:GLN:OE1	2.01	0.60
1:C:4:SER:OG	2:F:274:SER:OG	2.20	0.60
2:D:131:VAL:CG1	2:D:132:PRO:N	2.58	0.60
2:B:131:VAL:HG12	2:B:132:PRO:CD	2.30	0.60
1:E:112:LEU:CD2	2:F:72:MET:HG3	2.31	0.60
1:G:9:ASN:HD21	1:G:12:ASP:N	1.99	0.60
1:C:77:ARG:NH2	2:D:16:SER:O	2.34	0.60
2:B:142:LEU:HD12	2:B:146:LYS:CG	2.30	0.60
1:E:77:ARG:CD	2:F:15:GLU:HG2	2.31	0.60
2:H:431:VAL:HG22	2:H:441:PHE:HB2	1.83	0.60
2:D:142:LEU:HD12	2:D:146:LYS:CD	2.28	0.60
2:B:431:VAL:HG22	2:B:441:PHE:HB2	1.83	0.60
1:A:77:ARG:CZ	2:B:15:GLU:HB3	2.30	0.60
1:E:217:LEU:HD13	1:E:219:ASP:HB2	1.83	0.60
2:F:431:VAL:HG22	2:F:441:PHE:HB2	1.84	0.60
2:D:381:LEU:HD22	2:D:386:ILE:HD11	1.84	0.59
1:E:51:THR:CG2	2:F:83:ARG:HH11	2.15	0.59
1:A:112:LEU:CD1	2:B:76:LEU:CD2	2.80	0.59
1:E:97:ILE:HA	2:H:449:LEU:CD2	2.31	0.59
1:C:13:THR:CG2	2:D:5:ILE:CG2	2.72	0.59
1:E:190:LYS:HG3	1:E:191:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LYS:HG3	1:C:191:THR:O	2.02	0.59
2:D:431:VAL:HG22	2:D:441:PHE:HB2	1.84	0.59
1:G:296:MET:HG2	2:H:9:HIS:CD2	2.36	0.59
1:A:190:LYS:HG3	1:A:191:THR:O	2.02	0.59
2:B:381:LEU:HD22	2:B:386:ILE:HD11	1.84	0.59
2:B:382:SER:HB3	2:B:386:ILE:HD12	1.85	0.59
1:A:112:LEU:HD13	2:B:76:LEU:CD2	2.33	0.59
1:C:112:LEU:CD2	2:D:72:MET:CG	2.78	0.59
2:B:352:VAL:HG12	2:B:398:GLU:HG3	1.84	0.59
2:H:382:SER:HB3	2:H:386:ILE:HD12	1.85	0.59
2:H:141:ARG:O	2:H:145:HIS:HB2	2.03	0.59
1:C:49:LEU:HB3	2:D:128:ILE:N	2.17	0.59
1:G:9:ASN:ND2	1:G:12:ASP:H	2.01	0.59
2:B:141:ARG:O	2:B:145:HIS:HB2	2.03	0.59
2:D:131:VAL:HG12	2:D:132:PRO:CB	2.32	0.59
2:D:141:ARG:O	2:D:145:HIS:HB2	2.03	0.59
2:F:141:ARG:O	2:F:145:HIS:HB2	2.02	0.59
2:D:131:VAL:HG12	2:D:132:PRO:N	2.18	0.58
1:C:97:ILE:HA	2:F:449:LEU:CG	2.32	0.58
2:D:382:SER:HB3	2:D:386:ILE:HD12	1.85	0.58
2:F:352:VAL:HG12	2:F:398:GLU:HG3	1.84	0.58
1:E:110:PRO:HB3	2:F:132:PRO:CD	2.24	0.58
1:C:49:LEU:O	2:D:127:ALA:C	2.42	0.58
1:A:257:THR:HB	2:H:403:GLU:O	2.03	0.58
2:F:381:LEU:HD22	2:F:386:ILE:HD11	1.84	0.58
2:D:5:ILE:CG2	2:D:6:HIS:H	2.16	0.58
1:G:298:ILE:HD13	2:H:11:VAL:HG11	1.86	0.58
1:C:298:ILE:HD13	2:D:11:VAL:HG11	1.86	0.58
2:F:382:SER:HB3	2:F:386:ILE:HD12	1.85	0.58
1:A:110:PRO:HG3	2:B:135:ASP:OD1	2.03	0.58
2:F:5:ILE:CG2	2:F:6:HIS:H	2.16	0.58
1:G:79:SER:HB2	2:H:9:HIS:CG	2.39	0.58
1:E:79:SER:HB2	2:F:9:HIS:CG	2.39	0.58
1:C:158:ASN:HD22	1:C:159:ARG:N	1.97	0.58
1:C:9:ASN:ND2	1:C:12:ASP:H	2.01	0.58
2:H:381:LEU:HD22	2:H:386:ILE:HD11	1.84	0.58
1:C:321:ASP:OD1	1:C:326:ARG:HD2	2.04	0.58
1:C:101:GLN:NE2	1:C:138:ILE:HA	2.18	0.58
1:C:79:SER:HB2	2:D:9:HIS:CG	2.39	0.58
1:G:321:ASP:OD1	1:G:326:ARG:HD2	2.04	0.58
2:B:126:GLN:C	2:B:131:VAL:HG23	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:SER:HG	2:F:9:HIS:CE1	2.19	0.58
2:B:151:LEU:O	2:B:154:VAL:HG22	2.04	0.58
1:G:190:LYS:HG3	1:G:191:THR:O	2.02	0.58
1:E:321:ASP:OD1	1:E:326:ARG:HD2	2.04	0.58
2:F:151:LEU:O	2:F:154:VAL:HG22	2.04	0.58
1:E:77:ARG:HD2	2:F:15:GLU:CA	2.34	0.58
1:E:97:ILE:HA	2:H:449:LEU:HD22	1.86	0.58
1:A:13:THR:CG2	2:B:5:ILE:CG2	2.72	0.58
1:A:79:SER:HB2	2:B:9:HIS:CG	2.39	0.58
2:D:115:LEU:HD23	2:D:144:ALA:CB	2.31	0.58
2:H:151:LEU:O	2:H:154:VAL:HG22	2.04	0.58
2:H:352:VAL:HG12	2:H:398:GLU:HG3	1.84	0.58
1:E:101:GLN:NE2	1:E:138:ILE:HA	2.19	0.58
1:A:110:PRO:HB2	2:B:135:ASP:OD1	2.04	0.57
2:B:5:ILE:CG2	2:B:6:HIS:N	2.67	0.57
2:H:5:ILE:CG2	2:H:6:HIS:H	2.16	0.57
1:G:77:ARG:HD2	2:H:15:GLU:CA	2.34	0.57
2:D:3:VAL:CA	2:D:4:TYR:CB	2.82	0.57
2:D:5:ILE:CG2	2:D:6:HIS:N	2.67	0.57
1:E:298:ILE:HD13	2:F:11:VAL:HG11	1.86	0.57
2:D:352:VAL:HG12	2:D:398:GLU:HG3	1.84	0.57
2:D:69:ARG:HG3	2:D:133:TRP:CZ2	2.39	0.57
1:G:77:ARG:CD	2:H:136:LYS:NZ	2.68	0.57
2:D:351:LEU:HD12	2:D:399:LEU:HD12	1.87	0.57
2:D:126:GLN:HB3	2:D:131:VAL:HG21	1.86	0.57
2:B:131:VAL:HG12	2:B:132:PRO:N	2.18	0.57
2:H:143:ASP:O	2:H:144:ALA:CB	2.52	0.57
1:G:101:GLN:NE2	1:G:138:ILE:HA	2.19	0.57
2:B:132:PRO:CG	2:B:135:ASP:CA	2.67	0.57
2:F:131:VAL:HG12	2:F:132:PRO:N	2.18	0.57
1:A:9:ASN:HD21	1:A:12:ASP:N	1.99	0.57
1:A:245:LEU:HD12	2:B:68:LEU:HD23	1.84	0.57
1:A:321:ASP:OD1	1:A:326:ARG:HD2	2.03	0.57
1:A:112:LEU:CD2	2:B:76:LEU:HD22	2.33	0.57
1:A:49:LEU:CD1	2:B:367:GLU:HG3	2.25	0.57
2:B:143:ASP:O	2:B:144:ALA:CB	2.52	0.57
2:D:132:PRO:CG	2:D:135:ASP:CA	2.68	0.57
1:C:97:ILE:CA	2:F:449:LEU:HD11	2.27	0.57
2:B:351:LEU:HD12	2:B:399:LEU:HD12	1.86	0.57
2:F:126:GLN:HB3	2:F:131:VAL:HG21	1.86	0.57
1:E:112:LEU:CD1	2:F:76:LEU:CD2	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:ND2	1:A:12:ASP:H	2.01	0.57
2:D:151:LEU:O	2:D:154:VAL:HG22	2.04	0.57
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.19	0.57
2:F:351:LEU:HD12	2:F:399:LEU:HD12	1.87	0.57
2:D:141:ARG:O	2:D:146:LYS:HG2	1.90	0.57
2:H:131:VAL:HG12	2:H:132:PRO:N	2.18	0.57
2:F:126:GLN:C	2:F:131:VAL:HG23	2.18	0.57
2:F:5:ILE:CG2	2:F:6:HIS:N	2.67	0.57
2:H:351:LEU:HD12	2:H:399:LEU:HD12	1.86	0.57
2:H:16:SER:O	2:H:17:THR:CB	2.53	0.57
2:B:16:SER:O	2:B:17:THR:CB	2.53	0.57
1:G:79:SER:HG	2:H:9:HIS:CE1	2.20	0.57
2:F:143:ASP:O	2:F:144:ALA:CB	2.52	0.57
1:A:281:GLU:OE1	2:B:4:TYR:CE2	2.58	0.56
1:E:281:GLU:OE1	2:F:4:TYR:CE2	2.58	0.56
1:G:281:GLU:OE1	2:H:4:TYR:CE2	2.58	0.56
2:H:5:ILE:CG2	2:H:6:HIS:N	2.67	0.56
2:H:126:GLN:C	2:H:131:VAL:HG23	2.18	0.56
2:H:131:VAL:HG12	2:H:132:PRO:CB	2.33	0.56
2:B:69:ARG:HG3	2:B:133:TRP:CZ2	2.39	0.56
2:B:5:ILE:CG2	2:B:6:HIS:H	2.16	0.56
1:A:36:SER:HB3	2:B:12:ILE:HB	1.88	0.56
1:A:298:ILE:HD13	2:B:11:VAL:HG11	1.86	0.56
2:F:16:SER:O	2:F:17:THR:CB	2.53	0.56
1:C:251:LYS:NZ	1:C:285:SER:HB2	2.21	0.56
1:C:77:ARG:NE	2:D:136:LYS:NZ	2.54	0.56
1:A:77:ARG:HD2	2:B:15:GLU:CA	2.34	0.56
1:C:6:ILE:CG1	2:F:273:THR:HA	2.36	0.56
1:A:251:LYS:NZ	1:A:285:SER:HB2	2.21	0.56
2:F:346:LEU:HD23	2:F:347:THR:N	2.21	0.56
2:D:16:SER:O	2:D:17:THR:CB	2.53	0.56
1:E:110:PRO:HG3	2:F:135:ASP:CG	2.25	0.56
1:G:35:GLY:O	2:H:12:ILE:CG2	2.33	0.56
1:E:9:ASN:ND2	1:E:12:ASP:H	2.01	0.56
2:B:346:LEU:HD23	2:B:347:THR:N	2.21	0.56
1:E:251:LYS:NZ	1:E:285:SER:HB2	2.21	0.56
2:H:132:PRO:C	2:H:134:LYS:H	2.10	0.56
2:F:141:ARG:O	2:F:146:LYS:HG2	1.91	0.56
2:F:69:ARG:HG3	2:F:133:TRP:CZ2	2.39	0.56
1:C:110:PRO:CG	2:D:135:ASP:CG	2.67	0.56
2:F:3:VAL:CA	2:F:4:TYR:CB	2.82	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:ALA:O	2:D:218:ILE:HG22	2.06	0.56
2:H:126:GLN:HB3	2:H:131:VAL:HG21	1.86	0.55
1:C:281:GLU:OE1	2:D:4:TYR:CE2	2.58	0.55
1:E:112:LEU:HD13	2:F:76:LEU:HD22	1.88	0.55
2:H:439:LEU:HD22	2:H:442:LEU:HD21	1.88	0.55
1:C:101:GLN:HE22	1:C:138:ILE:HA	1.71	0.55
1:A:211:GLU:H	1:A:211:GLU:CD	2.10	0.55
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.88	0.55
2:H:215:ALA:O	2:H:218:ILE:HG22	2.06	0.55
2:D:132:PRO:C	2:D:134:LYS:H	2.09	0.55
1:E:77:ARG:HD3	2:F:136:LYS:NZ	2.21	0.55
1:C:211:GLU:CD	1:C:211:GLU:H	2.10	0.55
1:E:43:SER:HB2	1:E:105:GLU:HB3	1.88	0.55
1:E:211:GLU:H	1:E:211:GLU:CD	2.10	0.55
1:C:36:SER:HB3	2:D:12:ILE:HB	1.88	0.55
1:G:36:SER:HB3	2:H:12:ILE:HB	1.88	0.55
2:D:118:LEU:HD11	2:D:379:GLN:OE1	2.07	0.55
2:F:215:ALA:O	2:F:218:ILE:HG22	2.06	0.55
1:C:298:ILE:O	1:C:303:GLY:HA3	2.07	0.55
2:H:118:LEU:HD11	2:H:379:GLN:OE1	2.07	0.55
2:D:84:ILE:HD13	2:D:362:LEU:HD11	1.89	0.55
1:G:101:GLN:HE22	1:G:138:ILE:HA	1.71	0.55
2:H:153:ALA:O	2:H:157:LEU:HD23	2.07	0.55
2:B:153:ALA:O	2:B:157:LEU:HD23	2.07	0.55
2:B:215:ALA:O	2:B:218:ILE:HG22	2.06	0.55
2:F:131:VAL:HG12	2:F:132:PRO:CB	2.32	0.55
1:A:298:ILE:O	1:A:303:GLY:HA3	2.07	0.55
2:F:84:ILE:HD13	2:F:362:LEU:HD11	1.89	0.55
1:A:143:ILE:HD13	1:A:151:ASP:OD2	2.07	0.55
2:H:346:LEU:HD23	2:H:347:THR:N	2.21	0.55
1:G:251:LYS:NZ	1:G:285:SER:HB2	2.21	0.55
1:G:211:GLU:CD	1:G:211:GLU:H	2.10	0.55
1:G:51:THR:HG21	2:H:83:ARG:NH1	2.20	0.55
1:A:51:THR:CG2	2:B:83:ARG:HH11	2.18	0.55
2:D:118:LEU:HD11	2:D:379:GLN:HG3	1.89	0.55
2:H:84:ILE:HD13	2:H:362:LEU:HD11	1.89	0.55
2:D:346:LEU:HD23	2:D:347:THR:N	2.21	0.55
2:F:153:ALA:O	2:F:157:LEU:HD23	2.07	0.55
1:E:273:THR:HG22	1:E:274:SER:N	2.22	0.55
2:F:118:LEU:HD11	2:F:379:GLN:OE1	2.07	0.55
2:F:439:LEU:HD22	2:F:442:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:ALA:O	2:D:157:LEU:HD23	2.07	0.55
1:A:225:ILE:HG13	1:A:311:THR:HB	1.89	0.55
1:C:6:ILE:HG13	2:F:273:THR:HA	1.89	0.55
1:A:255:GLY:HA3	1:A:280:GLN:HE22	1.72	0.55
1:C:225:ILE:HG13	1:C:311:THR:HB	1.89	0.55
1:A:112:LEU:HD11	2:B:76:LEU:HD22	1.88	0.55
1:C:143:ILE:HD13	1:C:151:ASP:OD2	2.07	0.55
1:E:298:ILE:O	1:E:303:GLY:HA3	2.07	0.54
1:G:255:GLY:HA3	1:G:280:GLN:HE22	1.72	0.54
2:F:118:LEU:HD11	2:F:379:GLN:HG3	1.89	0.54
2:H:277:VAL:HG13	2:H:278:PRO:HD2	1.89	0.54
2:H:142:LEU:CD1	2:H:146:LYS:CG	2.77	0.54
2:H:4:TYR:N	2:H:4:TYR:CD1	2.75	0.54
1:E:36:SER:HB3	2:F:12:ILE:HB	1.88	0.54
1:G:298:ILE:O	1:G:303:GLY:HA3	2.07	0.54
1:C:255:GLY:HA3	1:C:280:GLN:HE22	1.72	0.54
1:E:251:LYS:HZ1	1:E:285:SER:HB2	1.72	0.54
1:C:77:ARG:HD2	2:D:15:GLU:CA	2.34	0.54
2:B:126:GLN:HB3	2:B:131:VAL:HG21	1.86	0.54
2:D:4:TYR:N	2:D:4:TYR:CD1	2.75	0.54
2:B:118:LEU:HD11	2:B:379:GLN:OE1	2.07	0.54
1:G:43:SER:HB2	1:G:105:GLU:HB3	1.88	0.54
1:E:143:ILE:HD13	1:E:151:ASP:OD2	2.07	0.54
2:B:126:GLN:HA	2:B:131:VAL:HG23	1.87	0.54
2:F:115:LEU:HD23	2:F:144:ALA:CB	2.31	0.54
2:D:143:ASP:O	2:D:144:ALA:CB	2.52	0.54
2:B:439:LEU:HD22	2:B:442:LEU:HD21	1.88	0.54
2:B:243:LEU:HD11	2:B:245:PHE:HB2	1.90	0.54
1:C:43:SER:HB2	1:C:105:GLU:HB3	1.88	0.54
1:A:9:ASN:ND2	1:A:9:ASN:C	2.61	0.54
1:E:255:GLY:HA3	1:E:280:GLN:HE22	1.72	0.54
1:A:215:LEU:N	1:A:215:LEU:HD12	2.23	0.54
1:C:215:LEU:N	1:C:215:LEU:HD12	2.23	0.54
2:B:333:LEU:N	2:B:333:LEU:HD13	2.23	0.54
2:F:243:LEU:HD11	2:F:245:PHE:HB2	1.90	0.54
1:A:226:SER:OG	1:A:307:ALA:HB3	2.08	0.54
1:E:9:ASN:C	1:E:9:ASN:ND2	2.61	0.54
1:E:244:ARG:HD2	1:E:249:VAL:HG13	1.90	0.54
2:F:277:VAL:HG13	2:F:278:PRO:HD2	1.89	0.54
2:B:131:VAL:HG12	2:B:132:PRO:CB	2.33	0.54
2:B:4:TYR:N	2:B:4:TYR:CD1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:THR:CG2	2:H:5:ILE:CG2	2.72	0.54
2:H:115:LEU:HD23	2:H:144:ALA:CB	2.31	0.54
1:A:211:GLU:O	1:A:212:ASP:HB2	2.08	0.54
1:C:211:GLU:O	1:C:212:ASP:HB2	2.08	0.54
1:C:51:THR:HG21	2:D:83:ARG:HH11	1.72	0.54
2:D:126:GLN:C	2:D:131:VAL:HG23	2.18	0.54
2:F:126:GLN:C	2:F:131:VAL:HB	2.28	0.54
2:F:132:PRO:C	2:F:134:LYS:H	2.09	0.54
2:D:449:LEU:CD2	1:G:97:ILE:HA	2.38	0.54
1:C:244:ARG:HD2	1:C:249:VAL:HG13	1.90	0.54
1:A:244:ARG:HD2	1:A:249:VAL:HG13	1.90	0.54
2:D:439:LEU:HD22	2:D:442:LEU:HD21	1.88	0.54
1:C:226:SER:OG	1:C:307:ALA:HB3	2.08	0.54
2:H:243:LEU:HD11	2:H:245:PHE:HB2	1.90	0.54
2:B:126:GLN:C	2:B:131:VAL:HB	2.28	0.54
1:G:99:VAL:HG11	1:G:142:ILE:HG12	1.90	0.54
2:F:441:PHE:C	2:F:442:LEU:HD22	2.29	0.54
1:E:211:GLU:O	1:E:212:ASP:HB2	2.08	0.54
2:D:126:GLN:C	2:D:131:VAL:HB	2.28	0.53
2:H:126:GLN:C	2:H:131:VAL:HB	2.28	0.53
2:F:135:ASP:O	2:F:136:LYS:CG	2.57	0.53
1:A:101:GLN:HE22	1:A:138:ILE:HA	1.71	0.53
2:B:277:VAL:HG13	2:B:278:PRO:HD2	1.89	0.53
2:B:132:PRO:C	2:B:134:LYS:H	2.10	0.53
1:E:99:VAL:HG11	1:E:142:ILE:HG12	1.90	0.53
1:E:215:LEU:N	1:E:215:LEU:HD12	2.23	0.53
2:B:135:ASP:O	2:B:136:LYS:CG	2.57	0.53
1:G:273:THR:HG22	1:G:274:SER:N	2.22	0.53
2:H:118:LEU:HD11	2:H:379:GLN:HG3	1.89	0.53
2:D:333:LEU:N	2:D:333:LEU:HD13	2.23	0.53
2:B:441:PHE:C	2:B:442:LEU:HD22	2.29	0.53
2:D:441:PHE:C	2:D:442:LEU:HD22	2.29	0.53
2:D:277:VAL:HG13	2:D:278:PRO:HD2	1.89	0.53
1:C:77:ARG:NE	2:D:136:LYS:HZ3	2.07	0.53
1:C:98:THR:OG1	2:F:449:LEU:HD23	2.08	0.53
2:F:3:VAL:HB	2:F:4:TYR:HD2	1.62	0.53
1:A:112:LEU:HD23	2:B:72:MET:HG3	1.89	0.53
1:G:211:GLU:O	1:G:212:ASP:HB2	2.08	0.53
1:G:226:SER:OG	1:G:307:ALA:HB3	2.08	0.53
2:B:9:HIS:CE1	2:B:11:VAL:CG2	2.92	0.53
1:E:225:ILE:HG13	1:E:311:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:LEU:HD11	2:D:245:PHE:HB2	1.90	0.53
1:G:215:LEU:N	1:G:215:LEU:HD12	2.23	0.53
1:G:143:ILE:HD13	1:G:151:ASP:OD2	2.07	0.53
2:H:69:ARG:HG3	2:H:133:TRP:CZ2	2.39	0.53
1:E:226:SER:OG	1:E:307:ALA:HB3	2.08	0.53
1:E:77:ARG:CZ	2:F:136:LYS:HZ3	2.21	0.53
1:C:273:THR:HG22	1:C:274:SER:N	2.22	0.53
1:A:99:VAL:HG11	1:A:142:ILE:HG12	1.90	0.53
2:H:441:PHE:C	2:H:442:LEU:HD22	2.29	0.53
2:B:118:LEU:HD11	2:B:379:GLN:HG3	1.89	0.53
1:C:251:LYS:HZ1	1:C:285:SER:HB2	1.72	0.53
1:G:225:ILE:HG13	1:G:311:THR:HB	1.89	0.53
2:H:126:GLN:HA	2:H:131:VAL:HG23	1.87	0.53
1:G:9:ASN:ND2	1:G:9:ASN:C	2.61	0.53
2:F:333:LEU:HD13	2:F:333:LEU:N	2.23	0.53
2:B:84:ILE:HD13	2:B:362:LEU:HD11	1.89	0.53
2:H:333:LEU:HD13	2:H:333:LEU:N	2.23	0.53
1:C:99:VAL:HG11	1:C:142:ILE:HG12	1.90	0.53
2:D:298:VAL:HG22	2:D:312:ILE:HA	1.91	0.53
1:C:27:THR:O	1:C:57:LYS:HG2	2.09	0.53
1:G:77:ARG:CD	2:H:136:LYS:HZ3	2.22	0.52
2:B:141:ARG:O	2:B:146:LYS:HG2	1.91	0.52
2:F:84:ILE:O	2:F:91:LEU:HD21	2.09	0.52
1:A:49:LEU:HB3	2:B:127:ALA:HB3	1.91	0.52
1:G:244:ARG:HD2	1:G:249:VAL:HG13	1.90	0.52
1:E:101:GLN:HE22	1:E:138:ILE:HA	1.71	0.52
2:H:298:VAL:HG22	2:H:312:ILE:HA	1.92	0.52
2:F:4:TYR:CD1	2:F:4:TYR:N	2.75	0.52
2:D:9:HIS:CE1	2:D:11:VAL:CG2	2.92	0.52
2:D:84:ILE:O	2:D:91:LEU:HD21	2.09	0.52
1:C:161:SER:OG	1:C:162:GLU:N	2.42	0.52
2:B:298:VAL:HG22	2:B:312:ILE:HA	1.91	0.52
1:C:77:ARG:CZ	2:D:136:LYS:HZ3	2.22	0.52
1:A:273:THR:HG22	1:A:274:SER:N	2.22	0.52
2:H:84:ILE:O	2:H:91:LEU:HD21	2.09	0.52
2:D:125:LEU:O	2:D:129:LEU:HG	2.09	0.52
2:F:125:LEU:O	2:F:129:LEU:HG	2.09	0.52
2:H:74:GLY:HA3	2:H:438:ALA:HB2	1.91	0.52
2:F:74:GLY:HA3	2:F:438:ALA:HB2	1.92	0.52
2:H:3:VAL:CA	2:H:4:TYR:CB	2.82	0.52
2:H:9:HIS:CE1	2:H:11:VAL:CG2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:HZ1	1:A:285:SER:HB2	1.74	0.52
2:D:74:GLY:HA3	2:D:438:ALA:HB2	1.92	0.52
1:A:27:THR:O	1:A:57:LYS:HG2	2.09	0.52
1:A:245:LEU:HD12	2:B:68:LEU:CD2	2.12	0.52
2:F:9:HIS:CE1	2:F:11:VAL:CG2	2.92	0.52
2:F:298:VAL:HG22	2:F:312:ILE:HA	1.91	0.52
1:A:79:SER:HG	2:B:9:HIS:CE1	2.22	0.52
1:G:27:THR:O	1:G:57:LYS:HG2	2.09	0.52
2:D:135:ASP:O	2:D:136:LYS:CG	2.57	0.52
2:D:142:LEU:CD1	2:D:146:LYS:CG	2.77	0.51
2:D:272:SER:O	1:G:6:ILE:CD1	2.57	0.51
1:A:51:THR:CG2	2:B:83:ARG:HG2	2.07	0.51
1:C:49:LEU:HB3	2:D:127:ALA:C	2.30	0.51
1:C:49:LEU:CD1	2:D:367:GLU:HG3	2.19	0.51
2:B:115:LEU:HD23	2:B:144:ALA:CB	2.31	0.51
1:G:206:SER:O	1:G:208:LEU:HG	2.11	0.51
2:H:125:LEU:O	2:H:129:LEU:HG	2.09	0.51
2:H:135:ASP:O	2:H:136:LYS:CG	2.57	0.51
2:H:142:LEU:CD1	2:H:146:LYS:CD	2.88	0.51
1:C:23:THR:CG2	2:F:95:VAL:HG23	2.38	0.51
1:C:206:SER:O	1:C:208:LEU:HG	2.11	0.51
2:D:69:ARG:NH1	2:D:133:TRP:CZ2	2.79	0.51
1:G:112:LEU:HD21	2:H:76:LEU:CD2	2.36	0.51
1:A:79:SER:HB2	2:B:9:HIS:ND1	2.24	0.51
1:C:10:TYR:CG	1:C:118:GLU:HG3	2.46	0.51
1:A:206:SER:O	1:A:208:LEU:HG	2.11	0.51
1:E:27:THR:O	1:E:57:LYS:HG2	2.09	0.51
1:E:77:ARG:CD	2:F:136:LYS:HZ1	2.22	0.51
2:B:403:GLU:O	1:G:257:THR:CB	2.58	0.51
1:G:251:LYS:O	1:G:254:GLU:HG3	2.11	0.51
2:H:114:TYR:HB2	2:H:129:LEU:HD11	1.93	0.51
2:B:74:GLY:CA	2:B:438:ALA:HB2	2.41	0.51
2:B:125:LEU:O	2:B:129:LEU:HG	2.09	0.51
2:B:69:ARG:NH1	2:B:133:TRP:CZ2	2.79	0.51
2:B:3:VAL:CA	2:B:4:TYR:CB	2.82	0.51
2:D:144:ALA:O	2:D:148:LEU:CG	2.59	0.51
2:B:84:ILE:O	2:B:91:LEU:HD21	2.09	0.51
1:A:251:LYS:O	1:A:254:GLU:HG3	2.11	0.51
1:A:161:SER:OG	1:A:162:GLU:N	2.42	0.51
1:A:10:TYR:CG	1:A:118:GLU:HG3	2.46	0.51
2:H:74:GLY:CA	2:H:438:ALA:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:SER:OG	1:G:162:GLU:N	2.42	0.51
2:B:142:LEU:CD1	2:B:146:LYS:CD	2.88	0.51
2:B:82:PHE:CZ	2:B:333:LEU:HD23	2.46	0.51
1:C:251:LYS:O	1:C:254:GLU:HG3	2.11	0.51
2:B:123:ASP:HA	2:B:126:GLN:CD	2.31	0.51
2:F:142:LEU:CD1	2:F:146:LYS:CD	2.87	0.51
1:E:224:TYR:CD2	2:F:7:PRO:HB3	2.46	0.51
1:G:273:THR:CG2	1:G:274:SER:N	2.74	0.51
2:F:114:TYR:HB2	2:F:129:LEU:HD11	1.93	0.51
2:D:74:GLY:CA	2:D:438:ALA:HB2	2.41	0.51
2:B:74:GLY:HA3	2:B:438:ALA:HB2	1.92	0.51
1:E:161:SER:OG	1:E:162:GLU:N	2.42	0.51
2:H:377:ASN:C	2:H:378:LEU:HD12	2.32	0.51
1:C:273:THR:CG2	1:C:274:SER:N	2.74	0.51
2:D:82:PHE:CZ	2:D:333:LEU:HD23	2.46	0.51
2:D:142:LEU:CD1	2:D:146:LYS:CD	2.88	0.50
1:G:77:ARG:HD3	2:H:136:LYS:HZ1	1.75	0.50
1:G:79:SER:HB2	2:H:9:HIS:ND1	2.24	0.50
1:C:79:SER:CB	2:D:9:HIS:CG	2.94	0.50
1:C:79:SER:HG	2:D:9:HIS:CE1	2.25	0.50
1:C:79:SER:HB2	2:D:9:HIS:ND1	2.24	0.50
2:B:144:ALA:O	2:B:148:LEU:CG	2.59	0.50
1:C:9:ASN:C	1:C:9:ASN:ND2	2.61	0.50
2:H:314:PRO:HG3	2:H:320:LEU:HD22	1.93	0.50
1:E:206:SER:O	1:E:208:LEU:HG	2.11	0.50
2:B:114:TYR:HB2	2:B:129:LEU:HD11	1.93	0.50
2:B:377:ASN:C	2:B:378:LEU:HD12	2.32	0.50
1:C:77:ARG:CD	2:D:136:LYS:NZ	2.74	0.50
1:E:10:TYR:CG	1:E:118:GLU:HG3	2.46	0.50
1:A:273:THR:CG2	1:A:274:SER:N	2.74	0.50
1:G:10:TYR:CG	1:G:118:GLU:HG3	2.46	0.50
1:A:224:TYR:CD2	2:B:7:PRO:HB3	2.46	0.50
2:D:114:TYR:HB2	2:D:129:LEU:HD11	1.93	0.50
1:C:49:LEU:HB2	2:D:127:ALA:HB3	1.94	0.50
1:G:79:SER:CB	2:H:9:HIS:CG	2.94	0.50
1:A:79:SER:CB	2:B:9:HIS:CG	2.94	0.50
1:E:79:SER:HB2	2:F:9:HIS:ND1	2.24	0.50
2:F:82:PHE:CZ	2:F:333:LEU:HD23	2.46	0.50
2:F:74:GLY:CA	2:F:438:ALA:HB2	2.41	0.50
2:H:123:ASP:HA	2:H:126:GLN:CD	2.31	0.50
2:D:449:LEU:HD21	1:G:97:ILE:C	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:TYR:CD2	2:H:7:PRO:HB3	2.46	0.50
1:E:273:THR:CG2	1:E:274:SER:N	2.74	0.50
1:G:264:HIS:HE1	1:G:267:GLY:HA2	1.77	0.50
1:A:77:ARG:NE	2:B:136:LYS:HZ3	2.10	0.50
1:C:35:GLY:O	2:D:12:ILE:CG2	2.34	0.50
1:C:224:TYR:CD2	2:D:7:PRO:HB3	2.46	0.50
2:B:157:LEU:HD13	2:B:436:ALA:HB2	1.94	0.50
2:F:157:LEU:HD13	2:F:436:ALA:HB2	1.93	0.50
2:D:171:LEU:HD23	2:D:172:LEU:N	2.27	0.50
2:D:123:ASP:HA	2:D:126:GLN:CD	2.31	0.50
1:E:251:LYS:O	1:E:254:GLU:HG3	2.11	0.50
2:F:243:LEU:HD13	2:F:244:ALA:N	2.27	0.50
2:B:171:LEU:HD23	2:B:172:LEU:N	2.27	0.50
2:D:377:ASN:C	2:D:378:LEU:HD12	2.32	0.50
2:F:144:ALA:O	2:F:148:LEU:CG	2.59	0.50
1:C:10:TYR:CD1	1:C:118:GLU:HG3	2.47	0.50
2:H:82:PHE:CZ	2:H:333:LEU:HD23	2.46	0.50
1:A:205:SER:O	1:A:206:SER:HB3	2.12	0.50
1:E:205:SER:O	1:E:206:SER:HB3	2.12	0.50
2:H:157:LEU:HD13	2:H:436:ALA:HB2	1.93	0.50
2:D:243:LEU:HD13	2:D:244:ALA:N	2.27	0.50
1:A:264:HIS:HE1	1:A:267:GLY:HA2	1.77	0.50
2:D:14:ASN:O	2:D:15:GLU:O	2.30	0.50
1:G:77:ARG:HD2	2:H:15:GLU:CG	2.42	0.50
2:F:69:ARG:NH1	2:F:133:TRP:CZ2	2.79	0.50
1:G:112:LEU:CG	2:H:76:LEU:HD21	2.42	0.50
1:A:49:LEU:O	2:B:127:ALA:C	2.49	0.50
1:G:10:TYR:CD1	1:G:118:GLU:HG3	2.47	0.50
2:F:314:PRO:HG3	2:F:320:LEU:HD22	1.93	0.50
2:D:314:PRO:HG3	2:D:320:LEU:HD22	1.93	0.50
2:B:243:LEU:HD13	2:B:244:ALA:N	2.27	0.50
1:E:264:HIS:HE1	1:E:267:GLY:HA2	1.77	0.50
1:A:110:PRO:HG3	2:B:135:ASP:CG	2.32	0.49
2:B:14:ASN:O	2:B:15:GLU:O	2.30	0.49
1:C:112:LEU:HD13	2:D:76:LEU:HD22	1.70	0.49
1:E:79:SER:CB	2:F:9:HIS:CG	2.94	0.49
1:G:205:SER:O	1:G:206:SER:HB3	2.12	0.49
1:A:10:TYR:CD1	1:A:118:GLU:HG3	2.47	0.49
2:B:314:PRO:HG3	2:B:320:LEU:HD22	1.93	0.49
1:C:77:ARG:HD2	2:D:15:GLU:CG	2.42	0.49
1:G:77:ARG:HH21	2:H:15:GLU:C	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:ASP:HA	2:F:126:GLN:CD	2.31	0.49
1:A:112:LEU:CD2	2:B:72:MET:HG3	2.43	0.49
1:C:205:SER:O	1:C:206:SER:HB3	2.12	0.49
2:F:377:ASN:C	2:F:378:LEU:HD12	2.32	0.49
2:D:258:PHE:O	2:D:401:ALA:HB1	2.13	0.49
2:D:175:VAL:CG1	2:D:200:VAL:HG11	2.42	0.49
2:H:243:LEU:HD13	2:H:244:ALA:N	2.27	0.49
2:H:258:PHE:O	2:H:401:ALA:HB1	2.13	0.49
2:B:258:PHE:O	2:B:401:ALA:HB1	2.13	0.49
2:H:175:VAL:CG1	2:H:200:VAL:HG11	2.42	0.49
2:F:171:LEU:HD23	2:F:172:LEU:N	2.27	0.49
2:H:14:ASN:O	2:H:15:GLU:O	2.30	0.49
2:D:157:LEU:HD13	2:D:436:ALA:HB2	1.93	0.49
2:F:175:VAL:CG1	2:F:200:VAL:HG11	2.42	0.49
2:H:39:ILE:HD11	2:H:217:LYS:HB3	1.95	0.49
1:E:112:LEU:HD11	2:F:76:LEU:HD22	1.90	0.49
2:B:9:HIS:CE1	2:B:11:VAL:HG21	2.48	0.49
2:D:9:HIS:CE1	2:D:11:VAL:HG21	2.48	0.49
2:H:144:ALA:O	2:H:148:LEU:CG	2.59	0.49
2:H:82:PHE:CE1	2:H:333:LEU:HD23	2.48	0.49
2:H:171:LEU:HD23	2:H:172:LEU:N	2.27	0.49
2:B:175:VAL:CG1	2:B:200:VAL:HG11	2.42	0.49
1:C:77:ARG:HD3	2:D:136:LYS:NZ	2.26	0.49
2:F:126:GLN:HA	2:F:131:VAL:HG23	1.87	0.49
1:E:10:TYR:CD1	1:E:118:GLU:HG3	2.47	0.49
2:B:110:LEU:HB3	2:B:129:LEU:HD22	1.55	0.49
2:F:39:ILE:HD11	2:F:217:LYS:HB3	1.95	0.49
2:F:329:GLN:H	2:F:333:LEU:HD11	1.78	0.49
2:D:392:LEU:HD23	2:D:393:ASN:N	2.28	0.49
2:D:303:PHE:HB2	2:D:307:ALA:HB3	1.95	0.49
2:D:39:ILE:HD11	2:D:217:LYS:HB3	1.95	0.49
2:F:14:ASN:O	2:F:15:GLU:O	2.30	0.48
1:G:112:LEU:HD23	2:H:72:MET:CG	2.30	0.48
2:F:82:PHE:CE1	2:F:333:LEU:HD23	2.48	0.48
2:B:329:GLN:H	2:B:333:LEU:HD11	1.78	0.48
1:G:232:ILE:HG13	1:G:295:ALA:HA	1.95	0.48
2:H:392:LEU:HD23	2:H:393:ASN:N	2.28	0.48
2:F:392:LEU:HD23	2:F:393:ASN:N	2.28	0.48
1:A:77:ARG:HH21	2:B:15:GLU:C	2.16	0.48
1:A:112:LEU:HD13	2:B:76:LEU:HD13	1.95	0.48
2:H:275:VAL:HG12	2:H:277:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:SER:OG	1:G:49:LEU:HD23	2.13	0.48
2:D:329:GLN:H	2:D:333:LEU:HD11	1.78	0.48
2:D:82:PHE:CE1	2:D:333:LEU:HD23	2.48	0.48
2:B:82:PHE:CE1	2:B:333:LEU:HD23	2.48	0.48
2:D:275:VAL:HG12	2:D:277:VAL:HG23	1.96	0.48
2:H:329:GLN:H	2:H:333:LEU:HD11	1.78	0.48
2:F:258:PHE:O	2:F:401:ALA:HB1	2.13	0.48
2:F:159:VAL:HA	2:F:170:LEU:HD21	1.96	0.48
1:E:281:GLU:OE1	2:F:4:TYR:CZ	2.67	0.48
1:G:281:GLU:OE1	2:H:4:TYR:CZ	2.67	0.48
1:A:47:SER:OG	1:A:49:LEU:HD23	2.13	0.48
2:H:161:GLN:CB	2:H:164:ALA:HB3	2.44	0.48
2:H:356:SER:HB3	2:H:392:LEU:HD21	1.96	0.48
1:E:232:ILE:HG13	1:E:295:ALA:HA	1.95	0.48
1:C:264:HIS:HE1	1:C:267:GLY:HA2	1.77	0.48
1:C:186:ILE:N	1:C:186:ILE:HD12	2.29	0.48
1:E:112:LEU:HD13	2:F:76:LEU:CD1	2.44	0.48
1:E:49:LEU:CD1	2:F:367:GLU:CG	2.74	0.48
1:G:112:LEU:HD13	2:H:76:LEU:HD11	1.95	0.48
1:E:127:PHE:CB	1:E:192:GLY:HA2	2.44	0.48
2:F:175:VAL:HG12	2:F:200:VAL:HG11	1.96	0.48
2:B:392:LEU:HD23	2:B:393:ASN:N	2.28	0.48
1:A:232:ILE:HG13	1:A:295:ALA:HA	1.96	0.48
1:E:110:PRO:HB2	2:F:135:ASP:OD1	2.11	0.48
2:H:3:VAL:HB	2:H:4:TYR:HD2	1.62	0.48
2:B:285:THR:CG2	2:B:343:THR:HG22	2.39	0.48
1:G:127:PHE:CB	1:G:192:GLY:HA2	2.44	0.48
2:B:159:VAL:HA	2:B:170:LEU:HD21	1.96	0.48
2:D:181:ALA:HB2	2:D:242:THR:HA	1.96	0.48
1:A:281:GLU:OE1	2:B:4:TYR:CZ	2.67	0.48
1:C:47:SER:OG	1:C:49:LEU:HD23	2.13	0.48
1:G:127:PHE:HB2	1:G:192:GLY:HA2	1.96	0.48
2:H:175:VAL:HG12	2:H:200:VAL:HG11	1.96	0.48
1:A:186:ILE:N	1:A:186:ILE:HD12	2.29	0.48
2:H:69:ARG:NH1	2:H:133:TRP:CZ2	2.79	0.48
1:C:281:GLU:OE1	2:D:4:TYR:CZ	2.67	0.48
2:H:9:HIS:CE1	2:H:11:VAL:HG21	2.48	0.48
1:A:127:PHE:CB	1:A:192:GLY:HA2	2.44	0.48
2:B:181:ALA:HB2	2:B:242:THR:HA	1.96	0.48
1:E:186:ILE:HD12	1:E:186:ILE:N	2.29	0.48
1:C:77:ARG:HH21	2:D:15:GLU:C	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:GLN:CB	2:F:164:ALA:HB3	2.44	0.47
2:B:175:VAL:HG12	2:B:200:VAL:HG11	1.96	0.47
2:B:356:SER:HB3	2:B:392:LEU:HD21	1.96	0.47
2:B:39:ILE:HD11	2:B:217:LYS:HB3	1.95	0.47
2:F:303:PHE:HB2	2:F:307:ALA:HB3	1.95	0.47
1:G:77:ARG:O	2:H:13:HIS:CE1	2.67	0.47
1:E:159:ARG:HH11	1:E:159:ARG:HG2	1.79	0.47
2:F:356:SER:HB3	2:F:392:LEU:HD21	1.96	0.47
2:B:303:PHE:HB2	2:B:307:ALA:HB3	1.95	0.47
1:E:35:GLY:O	2:F:12:ILE:CG2	2.33	0.47
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.79	0.47
2:B:441:PHE:O	2:B:442:LEU:HD22	2.14	0.47
2:F:158:LEU:HD12	2:F:440:HIS:CD2	2.49	0.47
2:H:288:HIS:HB2	2:H:299:THR:HG22	1.96	0.47
2:H:303:PHE:HB2	2:H:307:ALA:HB3	1.95	0.47
1:E:77:ARG:HD2	2:F:15:GLU:CG	2.42	0.47
1:E:77:ARG:NE	2:F:136:LYS:HZ3	2.13	0.47
1:E:47:SER:OG	1:E:49:LEU:HD23	2.14	0.47
2:D:277:VAL:HG21	2:D:448:PRO:HD2	1.97	0.47
2:H:181:ALA:HB2	2:H:242:THR:HA	1.96	0.47
1:C:232:ILE:HG13	1:C:295:ALA:HA	1.96	0.47
2:D:159:VAL:HA	2:D:170:LEU:HD21	1.96	0.47
1:C:77:ARG:O	2:D:13:HIS:CE1	2.67	0.47
1:E:77:ARG:O	2:F:13:HIS:CE1	2.67	0.47
2:F:9:HIS:CE1	2:F:11:VAL:HG21	2.48	0.47
2:B:161:GLN:CB	2:B:164:ALA:HB3	2.44	0.47
2:H:441:PHE:O	2:H:442:LEU:HD22	2.15	0.47
2:D:110:LEU:HB3	2:D:129:LEU:HD22	1.55	0.47
2:F:288:HIS:HB2	2:F:299:THR:HG22	1.96	0.47
2:F:43:THR:OG1	2:F:204:ARG:NH1	2.48	0.47
2:B:288:HIS:HB2	2:B:299:THR:HG22	1.96	0.47
1:G:186:ILE:N	1:G:186:ILE:HD12	2.29	0.47
1:G:110:PRO:HG3	2:H:135:ASP:CB	2.45	0.47
2:D:161:GLN:CB	2:D:164:ALA:HB3	2.44	0.47
1:A:127:PHE:HB2	1:A:192:GLY:HA2	1.96	0.47
2:B:275:VAL:HG12	2:B:277:VAL:HG23	1.95	0.47
2:D:158:LEU:HD12	2:D:440:HIS:CD2	2.49	0.47
2:D:288:HIS:HB2	2:D:299:THR:HG22	1.96	0.47
2:D:43:THR:OG1	2:D:204:ARG:NH1	2.48	0.47
1:C:159:ARG:HH11	1:C:159:ARG:HG2	1.79	0.47
2:F:441:PHE:O	2:F:442:LEU:HD22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:MET:HE1	2:B:399:LEU:HD13	1.96	0.47
2:F:179:PHE:CG	2:F:218:ILE:HD11	2.50	0.47
2:H:277:VAL:HG21	2:H:448:PRO:HD2	1.97	0.47
2:D:175:VAL:HG12	2:D:200:VAL:HG11	1.96	0.47
2:D:356:SER:HB3	2:D:392:LEU:HD21	1.96	0.47
2:B:158:LEU:HD12	2:B:440:HIS:CD2	2.49	0.47
1:E:203:VAL:HG22	1:E:261:ILE:HD12	1.97	0.47
2:H:159:VAL:HA	2:H:170:LEU:HD21	1.96	0.47
2:H:158:LEU:HD12	2:H:440:HIS:CD2	2.49	0.47
1:C:203:VAL:HG22	1:C:261:ILE:HD12	1.97	0.47
2:B:43:THR:OG1	2:B:204:ARG:NH1	2.48	0.47
2:F:181:ALA:HB2	2:F:242:THR:HA	1.96	0.47
2:D:441:PHE:O	2:D:442:LEU:HD22	2.15	0.47
2:F:277:VAL:HG21	2:F:448:PRO:HD2	1.97	0.47
1:A:203:VAL:HG22	1:A:261:ILE:HD12	1.97	0.47
2:D:447:ASN:ND2	1:G:96:GLY:O	2.48	0.47
1:E:23:THR:HG21	2:H:95:VAL:HG23	1.89	0.47
2:F:275:VAL:HG12	2:F:277:VAL:HG23	1.96	0.47
1:E:199:LYS:HD2	1:E:264:HIS:CE1	2.50	0.47
1:G:203:VAL:HG22	1:G:261:ILE:HD12	1.97	0.47
1:A:77:ARG:O	2:B:13:HIS:CE1	2.67	0.47
2:F:3:VAL:CA	2:F:4:TYR:CG	2.98	0.47
1:C:127:PHE:CB	1:C:192:GLY:HA2	2.44	0.47
1:E:68:LYS:HB2	1:E:89:GLN:HB3	1.97	0.47
2:H:36:PRO:HB2	2:H:204:ARG:HA	1.98	0.47
1:G:68:LYS:HB2	1:G:89:GLN:HB3	1.97	0.47
1:C:49:LEU:C	2:D:127:ALA:HB1	2.36	0.46
2:D:95:VAL:HB	1:G:23:THR:HG21	1.98	0.46
1:E:127:PHE:HB2	1:E:192:GLY:HA2	1.96	0.46
2:B:179:PHE:CG	2:B:218:ILE:HD11	2.50	0.46
1:A:68:LYS:HB2	1:A:89:GLN:HB3	1.97	0.46
2:B:137:ASN:OD1	2:B:143:ASP:OD2	2.34	0.46
2:H:255:MET:HE2	2:H:399:LEU:HD22	1.97	0.46
2:B:277:VAL:HG21	2:B:448:PRO:HD2	1.97	0.46
2:D:111:ALA:HA	2:D:129:LEU:HD13	1.97	0.46
2:D:36:PRO:HB2	2:D:204:ARG:HA	1.98	0.46
2:B:304:THR:O	2:B:306:SER:N	2.48	0.46
2:F:69:ARG:NH1	2:F:133:TRP:HH2	2.13	0.46
2:B:3:VAL:CA	2:B:4:TYR:CG	2.98	0.46
2:B:111:ALA:HA	2:B:129:LEU:HD13	1.97	0.46
2:D:159:VAL:O	2:D:159:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:LEU:H	2:F:68:LEU:HD21	1.78	0.46
1:A:35:GLY:O	2:B:12:ILE:CG2	2.33	0.46
2:D:179:PHE:CG	2:D:218:ILE:HD11	2.50	0.46
2:H:43:THR:OG1	2:H:204:ARG:NH1	2.48	0.46
1:C:68:LYS:HB2	1:C:89:GLN:HB3	1.97	0.46
1:E:77:ARG:CD	2:F:136:LYS:NZ	2.79	0.46
2:F:17:THR:HG23	2:F:136:LYS:NZ	2.31	0.46
2:F:137:ASN:OD1	2:F:143:ASP:OD2	2.34	0.46
1:G:48:ARG:HD3	1:G:48:ARG:HA	1.76	0.46
2:B:159:VAL:O	2:B:159:VAL:HG13	2.16	0.46
2:D:3:VAL:CA	2:D:4:TYR:CG	2.98	0.46
1:E:49:LEU:HB3	2:F:127:ALA:CB	2.46	0.46
1:G:159:ARG:HG2	1:G:159:ARG:HH11	1.79	0.46
2:H:159:VAL:O	2:H:159:VAL:HG13	2.16	0.46
2:D:16:SER:O	2:D:17:THR:OG1	2.34	0.46
1:A:77:ARG:HD2	2:B:15:GLU:CG	2.42	0.46
2:H:3:VAL:CA	2:H:4:TYR:CG	2.98	0.46
1:C:23:THR:OG1	1:C:91:ILE:HD11	2.16	0.46
2:F:255:MET:HE2	2:F:399:LEU:HD22	1.98	0.46
2:H:351:LEU:HD12	2:H:399:LEU:CD1	2.46	0.46
2:H:179:PHE:CG	2:H:218:ILE:HD11	2.50	0.46
2:D:181:ALA:HB1	2:D:182:PRO:CD	2.46	0.46
1:G:235:LEU:HD23	1:G:235:LEU:C	2.36	0.46
1:C:97:ILE:HA	2:F:449:LEU:HD21	1.75	0.46
1:E:112:LEU:CD2	2:F:76:LEU:HD22	2.42	0.46
1:C:49:LEU:HB2	2:D:127:ALA:CB	2.45	0.46
2:H:137:ASN:OD1	2:H:143:ASP:OD2	2.34	0.46
2:F:111:ALA:HA	2:F:129:LEU:HD13	1.97	0.46
1:E:290:THR:HG22	1:E:291:LEU:N	2.31	0.46
1:A:235:LEU:HD23	1:A:235:LEU:C	2.36	0.46
2:D:17:THR:O	2:D:18:CYS:C	2.54	0.46
1:E:77:ARG:HD2	2:F:15:GLU:CB	2.46	0.46
1:G:23:THR:OG1	1:G:91:ILE:HD11	2.16	0.46
1:A:245:LEU:CD1	2:B:68:LEU:HD22	2.18	0.46
1:E:235:LEU:HD23	1:E:235:LEU:C	2.36	0.46
2:H:14:ASN:O	2:H:15:GLU:C	2.54	0.45
1:E:36:SER:CB	2:F:12:ILE:HB	2.46	0.45
1:G:49:LEU:HB2	2:H:127:ALA:HB3	1.96	0.45
1:A:199:LYS:HD2	1:A:264:HIS:CE1	2.50	0.45
1:C:199:LYS:HD2	1:C:264:HIS:CE1	2.50	0.45
2:D:158:LEU:HD23	2:D:159:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:230:THR:HG21	2:F:248:TYR:CD1	2.51	0.45
2:H:16:SER:O	2:H:17:THR:OG1	2.34	0.45
1:A:77:ARG:HD2	2:B:15:GLU:CB	2.46	0.45
2:B:17:THR:O	2:B:18:CYS:C	2.54	0.45
1:G:199:LYS:HD2	1:G:264:HIS:CE1	2.50	0.45
1:A:290:THR:HG22	1:A:291:LEU:N	2.31	0.45
2:D:230:THR:HG21	2:D:248:TYR:CD1	2.51	0.45
2:D:230:THR:HG21	2:D:248:TYR:HD1	1.82	0.45
1:C:235:LEU:HD23	1:C:235:LEU:C	2.37	0.45
2:D:131:VAL:HG12	2:D:132:PRO:HB3	1.91	0.45
2:H:111:ALA:HA	2:H:129:LEU:HD13	1.98	0.45
2:F:158:LEU:HD23	2:F:159:VAL:N	2.31	0.45
2:F:159:VAL:HG13	2:F:159:VAL:O	2.16	0.45
2:B:181:ALA:HB1	2:B:182:PRO:CD	2.46	0.45
2:B:36:PRO:HB2	2:B:204:ARG:HA	1.97	0.45
2:H:230:THR:HG21	2:H:248:TYR:HD1	1.82	0.45
2:F:131:VAL:HG12	2:F:132:PRO:HD3	1.99	0.45
1:A:36:SER:CB	2:B:12:ILE:HB	2.46	0.45
1:E:11:MET:O	1:E:12:ASP:HB2	2.17	0.45
2:D:151:LEU:HD12	2:D:154:VAL:HG21	1.98	0.45
2:F:36:PRO:HB2	2:F:204:ARG:HA	1.98	0.45
2:H:230:THR:HG21	2:H:248:TYR:CD1	2.51	0.45
2:B:14:ASN:O	2:B:15:GLU:C	2.54	0.45
2:D:367:GLU:C	2:D:368:LEU:HD13	2.37	0.45
1:G:190:LYS:HD2	1:G:191:THR:H	1.82	0.45
2:D:255:MET:HE2	2:D:399:LEU:HD22	1.97	0.45
2:B:351:LEU:HD12	2:B:399:LEU:CD1	2.46	0.45
2:D:292:ILE:HD12	2:D:293:GLN:N	2.32	0.45
1:A:137:PRO:HD2	1:A:140:ASP:OD2	2.17	0.45
1:G:77:ARG:HD2	2:H:15:GLU:CB	2.46	0.45
2:H:131:VAL:CB	2:H:132:PRO:HA	2.36	0.45
1:E:77:ARG:HH21	2:F:15:GLU:C	2.16	0.45
1:G:36:SER:CB	2:H:12:ILE:HB	2.46	0.45
2:F:326:LEU:O	2:F:333:LEU:HD12	2.17	0.45
2:F:395:ILE:HD12	2:F:395:ILE:C	2.37	0.45
1:C:190:LYS:HD2	1:C:191:THR:H	1.82	0.45
2:F:151:LEU:HD12	2:F:154:VAL:HG21	1.98	0.45
2:B:158:LEU:HD23	2:B:159:VAL:N	2.31	0.45
2:H:158:LEU:HD23	2:H:159:VAL:N	2.31	0.45
2:F:181:ALA:HB1	2:F:182:PRO:CD	2.46	0.45
2:B:230:THR:HG21	2:B:248:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:THR:HG22	1:G:291:LEU:N	2.31	0.45
1:G:137:PRO:HD2	1:G:140:ASP:OD2	2.17	0.45
1:C:98:THR:H	2:F:449:LEU:CD2	2.12	0.45
1:E:23:THR:OG1	1:E:91:ILE:HD11	2.16	0.45
1:A:245:LEU:C	2:B:68:LEU:HD13	2.36	0.45
1:C:127:PHE:HB2	1:C:192:GLY:HA2	1.97	0.45
2:D:351:LEU:HD12	2:D:399:LEU:CD1	2.46	0.45
2:D:131:VAL:HG12	2:D:132:PRO:HD3	1.99	0.45
2:H:14:ASN:ND2	2:H:14:ASN:N	2.64	0.45
1:E:23:THR:HG21	2:H:95:VAL:CB	2.46	0.45
1:A:49:LEU:C	2:B:127:ALA:HB1	2.37	0.45
2:D:381:LEU:HD23	2:D:381:LEU:C	2.37	0.45
1:A:7:LEU:HD11	1:A:169:ILE:HG13	1.99	0.45
2:D:304:THR:O	2:D:306:SER:N	2.48	0.45
1:C:137:PRO:HD2	1:C:140:ASP:OD2	2.17	0.45
2:F:324:GLU:HG3	2:F:428:LEU:HD11	1.99	0.45
1:A:23:THR:OG1	1:A:91:ILE:HD11	2.16	0.45
1:C:77:ARG:HD2	2:D:15:GLU:CB	2.46	0.45
2:D:14:ASN:O	2:D:15:GLU:C	2.54	0.45
2:H:132:PRO:CD	2:H:135:ASP:HA	2.47	0.45
1:C:112:LEU:HD13	2:D:76:LEU:CD1	2.47	0.45
2:H:176:VAL:CG2	2:H:198:THR:HG21	2.46	0.45
2:B:395:ILE:C	2:B:395:ILE:HD12	2.37	0.45
1:E:190:LYS:HD2	1:E:191:THR:H	1.82	0.45
2:H:381:LEU:HD23	2:H:381:LEU:C	2.37	0.45
2:B:151:LEU:HD12	2:B:154:VAL:HG21	1.98	0.45
2:H:110:LEU:HB3	2:H:129:LEU:HD22	1.55	0.45
2:H:181:ALA:HB1	2:H:182:PRO:CD	2.46	0.45
2:B:292:ILE:HD12	2:B:293:GLN:N	2.32	0.45
2:D:37:ALA:HB1	2:D:38:PRO:HD2	1.98	0.45
2:D:126:GLN:HA	2:D:131:VAL:HG23	1.87	0.45
2:F:17:THR:CG2	2:F:136:LYS:HD3	2.47	0.45
2:D:395:ILE:C	2:D:395:ILE:HD12	2.37	0.45
2:F:175:VAL:HG12	2:F:200:VAL:CB	2.47	0.45
1:E:137:PRO:HD2	1:E:140:ASP:OD2	2.17	0.45
1:C:290:THR:HG22	1:C:291:LEU:N	2.31	0.45
2:F:14:ASN:O	2:F:15:GLU:C	2.54	0.44
2:D:326:LEU:O	2:D:333:LEU:HD12	2.17	0.44
2:B:230:THR:HG21	2:B:248:TYR:HD1	1.82	0.44
1:G:7:LEU:HD11	1:G:169:ILE:HG13	1.99	0.44
2:H:292:ILE:HD12	2:H:293:GLN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:OG1	2:B:136:LYS:HE3	2.18	0.44
1:C:36:SER:CB	2:D:12:ILE:HB	2.46	0.44
2:F:367:GLU:C	2:F:368:LEU:HD13	2.37	0.44
2:D:95:VAL:CG2	1:G:23:THR:HG21	2.47	0.44
1:A:11:MET:O	1:A:12:ASP:HB2	2.17	0.44
2:B:326:LEU:O	2:B:333:LEU:CD1	2.66	0.44
2:H:255:MET:HE3	2:H:399:LEU:HB3	1.99	0.44
2:B:312:ILE:HG21	2:B:327:THR:HG21	1.99	0.44
2:H:17:THR:O	2:H:18:CYS:C	2.54	0.44
2:F:17:THR:O	2:F:18:CYS:C	2.54	0.44
2:B:121:THR:HA	2:B:372:LEU:HD11	2.00	0.44
2:H:367:GLU:C	2:H:368:LEU:HD13	2.37	0.44
2:D:137:ASN:OD1	2:D:143:ASP:OD2	2.34	0.44
2:D:285:THR:CG2	2:D:343:THR:HG22	2.39	0.44
2:B:326:LEU:O	2:B:333:LEU:HD12	2.17	0.44
1:A:190:LYS:HD2	1:A:191:THR:H	1.82	0.44
2:F:255:MET:HE3	2:F:399:LEU:HB3	1.99	0.44
1:G:151:ASP:O	1:G:322:ARG:HB2	2.18	0.44
2:B:175:VAL:HG12	2:B:200:VAL:CB	2.47	0.44
2:H:428:LEU:HD13	2:H:444:ARG:HA	1.99	0.44
1:E:7:LEU:HD11	1:E:169:ILE:HG13	1.99	0.44
2:D:132:PRO:C	2:D:134:LYS:N	2.70	0.44
2:B:132:PRO:CD	2:B:135:ASP:HA	2.47	0.44
2:B:367:GLU:C	2:B:368:LEU:HD13	2.37	0.44
2:F:285:THR:CG2	2:F:343:THR:HG22	2.39	0.44
1:G:244:ARG:HD2	1:G:249:VAL:CG1	2.48	0.44
2:B:324:GLU:HG3	2:B:428:LEU:HD11	1.99	0.44
2:B:37:ALA:HB1	2:B:38:PRO:HD2	1.99	0.44
1:C:299:PRO:HA	1:C:300:PRO:HD3	1.84	0.44
1:C:110:PRO:HB3	2:D:135:ASP:OD1	2.07	0.44
1:A:109:MET:HA	1:A:110:PRO:HD2	1.86	0.44
2:F:16:SER:O	2:F:17:THR:OG1	2.34	0.44
2:D:121:THR:HA	2:D:372:LEU:HD11	2.00	0.44
2:B:381:LEU:HD23	2:B:381:LEU:C	2.37	0.44
2:F:351:LEU:HD12	2:F:399:LEU:CD1	2.46	0.44
2:H:175:VAL:HG12	2:H:200:VAL:CB	2.47	0.44
2:D:131:VAL:CB	2:D:132:PRO:HA	2.36	0.44
2:H:326:LEU:O	2:H:333:LEU:HD12	2.17	0.44
2:F:381:LEU:HD23	2:F:381:LEU:C	2.37	0.44
2:D:175:VAL:HG12	2:D:200:VAL:CB	2.47	0.44
2:F:37:ALA:HB1	2:F:38:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:HD11	1:C:169:ILE:HG13	1.99	0.44
2:H:37:ALA:HB1	2:H:38:PRO:HD2	1.99	0.44
2:F:132:PRO:CD	2:F:135:ASP:HA	2.47	0.44
2:F:17:THR:HG21	2:F:136:LYS:HD3	1.99	0.44
1:C:97:ILE:CA	2:F:449:LEU:HD22	2.38	0.44
2:D:4:TYR:HD1	2:D:5:ILE:H	1.66	0.44
1:C:112:LEU:CD1	2:D:76:LEU:HD21	2.38	0.44
1:E:151:ASP:O	1:E:322:ARG:HB2	2.18	0.44
2:F:312:ILE:HG21	2:F:327:THR:HG21	2.00	0.44
2:H:324:GLU:HG3	2:H:428:LEU:HD11	1.99	0.44
2:F:180:THR:HB	2:F:184:LEU:HD13	2.00	0.44
2:F:292:ILE:HD12	2:F:293:GLN:N	2.32	0.44
1:G:243:LYS:HB2	1:G:248:TYR:CE2	2.53	0.44
2:D:134:LYS:O	2:D:135:ASP:CB	2.65	0.44
2:F:132:PRO:C	2:F:134:LYS:N	2.70	0.44
2:F:131:VAL:CB	2:F:132:PRO:HA	2.36	0.44
2:B:124:ARG:HD3	2:B:372:LEU:HD13	2.00	0.44
1:G:224:TYR:CE2	1:G:294:HIS:CE1	3.06	0.44
1:G:11:MET:O	1:G:12:ASP:HB2	2.17	0.44
2:D:326:LEU:O	2:D:333:LEU:CD1	2.66	0.44
2:F:326:LEU:O	2:F:333:LEU:CD1	2.66	0.44
2:H:326:LEU:O	2:H:333:LEU:CD1	2.66	0.44
2:H:395:ILE:HD12	2:H:395:ILE:C	2.37	0.44
2:F:249:VAL:HG11	2:F:395:ILE:HG22	2.00	0.44
2:H:312:ILE:HG21	2:H:327:THR:HG21	1.99	0.44
2:H:110:LEU:HD21	2:H:125:LEU:HD22	2.00	0.44
2:F:230:THR:HG21	2:F:248:TYR:HD1	1.82	0.44
1:G:129:GLU:N	1:G:129:GLU:OE1	2.51	0.44
1:E:77:ARG:NE	2:F:136:LYS:NZ	2.66	0.44
1:A:49:LEU:CB	2:B:127:ALA:HB3	2.48	0.44
2:F:106:VAL:HG13	2:F:359:LEU:CD1	2.48	0.44
1:E:245:LEU:HA	2:F:68:LEU:HD11	0.87	0.44
2:F:428:LEU:HD13	2:F:444:ARG:HA	1.99	0.44
1:C:243:LYS:HB2	1:C:248:TYR:CE2	2.53	0.44
2:H:249:VAL:HG11	2:H:395:ILE:HG22	2.00	0.43
1:E:42:PRO:HB2	1:E:58:LEU:HD23	2.00	0.43
1:G:42:PRO:HB2	1:G:58:LEU:HD23	2.00	0.43
1:A:299:PRO:HA	1:A:300:PRO:HD3	1.84	0.43
1:A:49:LEU:HB3	2:B:127:ALA:CB	2.48	0.43
1:E:244:ARG:HD2	1:E:249:VAL:CG1	2.48	0.43
1:C:321:ASP:HB3	1:C:326:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:LEU:HD12	2:H:154:VAL:HG21	1.98	0.43
1:G:139:PHE:CE1	1:G:143:ILE:HD11	2.53	0.43
2:B:110:LEU:HD21	2:B:125:LEU:HD22	2.00	0.43
2:H:285:THR:CG2	2:H:343:THR:HG22	2.39	0.43
1:A:151:ASP:O	1:A:322:ARG:HB2	2.18	0.43
2:H:221:PHE:O	2:H:225:VAL:HG23	2.19	0.43
1:A:42:PRO:HB2	1:A:58:LEU:HD23	2.00	0.43
1:A:217:LEU:CD1	1:A:219:ASP:HB2	2.48	0.43
1:C:244:ARG:HD2	1:C:249:VAL:CG1	2.48	0.43
1:A:206:SER:O	1:A:208:LEU:N	2.50	0.43
2:D:255:MET:HE3	2:D:399:LEU:HB3	1.99	0.43
1:E:139:PHE:CE1	1:E:143:ILE:HD11	2.53	0.43
2:D:428:LEU:HD13	2:D:444:ARG:HA	1.99	0.43
1:E:243:LYS:HB2	1:E:248:TYR:CE2	2.53	0.43
1:C:299:PRO:HG2	2:D:13:HIS:HB2	2.01	0.43
1:E:112:LEU:HA	1:E:113:PRO:HA	1.80	0.43
1:C:49:LEU:CB	2:D:127:ALA:HB1	2.47	0.43
2:D:124:ARG:HD3	2:D:372:LEU:HD13	2.00	0.43
1:A:244:ARG:HD2	1:A:249:VAL:CG1	2.47	0.43
1:E:321:ASP:HB3	1:E:326:ARG:HG3	2.01	0.43
1:A:139:PHE:CE1	1:A:143:ILE:HD11	2.53	0.43
1:E:236:MET:HG3	1:E:248:TYR:CD2	2.54	0.43
2:D:221:PHE:O	2:D:225:VAL:HG23	2.19	0.43
2:F:304:THR:O	2:F:306:SER:N	2.48	0.43
2:D:180:THR:HB	2:D:184:LEU:HD13	2.00	0.43
2:B:279:MET:HB3	2:B:279:MET:HE3	1.90	0.43
2:B:16:SER:O	2:B:17:THR:OG1	2.34	0.43
2:F:4:TYR:HD1	2:F:5:ILE:H	1.66	0.43
1:E:49:LEU:HB3	2:F:127:ALA:HB3	2.00	0.43
2:F:124:ARG:O	2:F:128:ILE:HG13	2.19	0.43
2:D:201:VAL:HG12	2:D:203:PRO:HD3	2.01	0.43
2:B:180:THR:HB	2:B:184:LEU:HD13	2.00	0.43
1:E:48:ARG:HA	1:E:48:ARG:HD3	1.76	0.43
2:B:142:LEU:O	2:B:146:LYS:CB	2.64	0.43
1:C:6:ILE:HG12	2:F:273:THR:HA	2.00	0.43
2:H:124:ARG:O	2:H:128:ILE:HG13	2.19	0.43
2:H:148:LEU:HD22	2:H:197:TYR:HB2	2.01	0.43
2:D:249:VAL:HG11	2:D:395:ILE:HG22	2.00	0.43
2:B:175:VAL:HG12	2:B:200:VAL:HB	2.01	0.43
2:B:428:LEU:HD13	2:B:444:ARG:HA	1.99	0.43
2:D:324:GLU:HG3	2:D:428:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MET:HG3	1:A:248:TYR:CD2	2.54	0.43
1:A:243:LYS:HB2	1:A:248:TYR:CE2	2.53	0.43
2:D:14:ASN:N	2:D:14:ASN:ND2	2.65	0.43
2:D:3:VAL:C	2:D:4:TYR:CG	2.92	0.43
2:B:3:VAL:C	2:B:4:TYR:CG	2.92	0.43
2:B:4:TYR:HD1	2:B:5:ILE:H	1.66	0.43
2:F:72:MET:O	2:F:76:LEU:HD23	2.19	0.43
2:F:124:ARG:HD3	2:F:372:LEU:HD13	2.00	0.43
1:E:224:TYR:CE2	1:E:294:HIS:CE1	3.06	0.43
1:C:191:THR:HG22	1:C:192:GLY:N	2.34	0.43
2:D:179:PHE:CD2	2:D:218:ILE:HD11	2.54	0.43
2:B:102:SER:HB3	2:B:105:ALA:HB3	2.01	0.43
2:H:102:SER:HB3	2:H:105:ALA:HB3	2.01	0.43
2:H:304:THR:O	2:H:306:SER:N	2.48	0.43
2:B:131:VAL:CB	2:B:132:PRO:HA	2.36	0.43
2:F:14:ASN:ND2	2:F:14:ASN:N	2.65	0.43
2:F:121:THR:HA	2:F:372:LEU:HD11	2.00	0.43
1:C:11:MET:O	1:C:12:ASP:HB2	2.17	0.43
1:A:321:ASP:HB3	1:A:326:ARG:HG3	2.01	0.43
2:F:255:MET:HE1	2:F:399:LEU:HD13	2.01	0.43
2:B:179:PHE:CD2	2:B:218:ILE:HD11	2.54	0.43
1:C:139:PHE:CE1	1:C:143:ILE:HD11	2.53	0.43
1:C:151:ASP:O	1:C:322:ARG:HB2	2.18	0.43
2:D:312:ILE:HG21	2:D:327:THR:HG21	1.99	0.43
1:C:42:PRO:HB2	1:C:58:LEU:HD23	2.00	0.43
1:E:129:GLU:N	1:E:129:GLU:OE1	2.51	0.43
2:H:69:ARG:NH1	2:H:133:TRP:HH2	2.13	0.43
1:A:112:LEU:HD13	2:B:76:LEU:HD11	2.00	0.43
2:D:148:LEU:HD22	2:D:197:TYR:HB2	2.01	0.43
1:G:191:THR:HG22	1:G:192:GLY:N	2.34	0.43
1:A:129:GLU:N	1:A:129:GLU:OE1	2.51	0.43
2:D:132:PRO:CD	2:D:135:ASP:HA	2.47	0.42
1:E:294:HIS:HE1	2:F:7:PRO:HG3	1.77	0.42
1:G:70:ASN:ND2	1:G:102:MET:HE3	2.34	0.42
2:B:87:MET:SD	2:B:91:LEU:HD23	2.59	0.42
1:C:236:MET:HG3	1:C:248:TYR:CD2	2.54	0.42
2:H:180:THR:HB	2:H:184:LEU:HD13	2.00	0.42
2:D:124:ARG:O	2:D:128:ILE:HG13	2.19	0.42
2:H:72:MET:O	2:H:76:LEU:HD23	2.19	0.42
2:D:87:MET:SD	2:D:91:LEU:HD23	2.59	0.42
2:H:106:VAL:HG13	2:H:359:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:THR:HG22	1:E:192:GLY:N	2.34	0.42
1:A:77:ARG:NE	2:B:136:LYS:NZ	2.67	0.42
2:B:134:LYS:O	2:B:135:ASP:CB	2.65	0.42
2:F:142:LEU:O	2:F:146:LYS:CB	2.64	0.42
2:F:3:VAL:C	2:F:4:TYR:CG	2.92	0.42
2:H:121:THR:HA	2:H:372:LEU:HD11	2.00	0.42
1:C:217:LEU:CD1	1:C:219:ASP:HB2	2.47	0.42
2:D:54:GLN:O	2:D:58:VAL:HG23	2.20	0.42
2:D:102:SER:HB3	2:D:105:ALA:HB3	2.01	0.42
2:B:201:VAL:HG12	2:B:203:PRO:HD3	2.01	0.42
1:E:33:ASP:OD1	2:F:10:LEU:HB3	2.20	0.42
2:B:124:ARG:O	2:B:128:ILE:HG13	2.19	0.42
2:H:124:ARG:HD3	2:H:372:LEU:HD13	2.00	0.42
1:E:217:LEU:CD1	1:E:219:ASP:HB2	2.47	0.42
1:A:70:ASN:ND2	1:A:102:MET:HE3	2.34	0.42
2:H:179:PHE:CD2	2:H:218:ILE:HD11	2.54	0.42
2:F:48:GLU:HG2	2:F:171:LEU:HD11	2.01	0.42
2:H:201:VAL:HG12	2:H:203:PRO:HD3	2.01	0.42
2:H:16:SER:C	2:H:17:THR:OG1	2.58	0.42
2:H:4:TYR:HD1	2:H:5:ILE:H	1.66	0.42
2:H:48:GLU:HG2	2:H:171:LEU:HD11	2.01	0.42
1:G:236:MET:HG3	1:G:248:TYR:CE2	2.55	0.42
1:C:96:GLY:CA	2:F:447:ASN:ND2	2.81	0.42
2:F:87:MET:SD	2:F:91:LEU:HD23	2.59	0.42
2:D:106:VAL:O	2:D:109:THR:HG22	2.20	0.42
2:B:249:VAL:HG11	2:B:395:ILE:HG22	2.00	0.42
2:H:106:VAL:O	2:H:109:THR:HG22	2.20	0.42
1:A:191:THR:HG22	1:A:192:GLY:N	2.34	0.42
1:G:321:ASP:HB3	1:G:326:ARG:HG3	2.01	0.42
2:F:110:LEU:HD21	2:F:125:LEU:HD22	2.00	0.42
1:G:236:MET:HG3	1:G:248:TYR:CD2	2.54	0.42
1:E:236:MET:HG3	1:E:248:TYR:CE2	2.55	0.42
1:A:33:ASP:OD1	2:B:10:LEU:HB3	2.20	0.42
1:C:33:ASP:OD1	2:D:10:LEU:HB3	2.20	0.42
2:H:54:GLN:O	2:H:58:VAL:HG23	2.20	0.42
1:C:129:GLU:N	1:C:129:GLU:OE1	2.51	0.42
1:G:299:PRO:HG2	2:H:13:HIS:HB2	2.01	0.42
2:H:131:VAL:HG12	2:H:132:PRO:HD3	1.99	0.42
2:F:4:TYR:CE1	2:F:5:ILE:HD12	2.55	0.42
2:H:144:ALA:O	2:H:148:LEU:HD12	2.19	0.42
2:B:144:ALA:O	2:B:148:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:HIS:HE1	2:H:7:PRO:HG3	1.77	0.42
1:A:283:TYR:HB2	2:H:285:THR:HG23	2.02	0.42
2:D:255:MET:HE1	2:D:399:LEU:HD13	2.01	0.42
2:F:179:PHE:CD2	2:F:218:ILE:HD11	2.54	0.42
2:H:34:PHE:CZ	2:H:191:VAL:HG21	2.55	0.42
2:B:54:GLN:O	2:B:58:VAL:HG23	2.20	0.42
1:C:48:ARG:HA	1:C:48:ARG:HD3	1.76	0.42
2:H:301:VAL:O	2:H:301:VAL:HG13	2.20	0.42
2:B:16:SER:C	2:B:17:THR:OG1	2.58	0.42
1:A:112:LEU:HD21	2:B:76:LEU:HD22	1.99	0.42
2:B:72:MET:O	2:B:76:LEU:HD23	2.19	0.42
2:H:175:VAL:HG12	2:H:200:VAL:HB	2.01	0.42
1:A:236:MET:HG3	1:A:248:TYR:CE2	2.55	0.42
2:B:221:PHE:O	2:B:225:VAL:HG23	2.19	0.42
2:F:34:PHE:CZ	2:F:191:VAL:HG21	2.55	0.42
2:F:102:SER:HB3	2:F:105:ALA:HB3	2.01	0.42
1:A:299:PRO:HG2	2:B:13:HIS:HB2	2.01	0.42
2:F:144:ALA:O	2:F:148:LEU:HD12	2.19	0.42
1:C:278:VAL:HG21	1:C:280:GLN:NE2	2.35	0.42
2:H:87:MET:SD	2:H:91:LEU:HD23	2.59	0.42
2:B:106:VAL:HG13	2:B:359:LEU:CD1	2.48	0.42
2:B:255:MET:CE	2:B:399:LEU:HD13	2.50	0.42
2:F:255:MET:CE	2:F:399:LEU:HD13	2.50	0.42
2:D:110:LEU:HD21	2:D:125:LEU:HD22	2.00	0.42
2:D:175:VAL:HG12	2:D:200:VAL:HB	2.01	0.42
2:B:288:HIS:CG	2:B:299:THR:HG22	2.55	0.42
1:C:236:MET:HG3	1:C:248:TYR:CE2	2.55	0.42
2:H:132:PRO:C	2:H:134:LYS:N	2.70	0.42
2:F:148:LEU:HD22	2:F:197:TYR:HB2	2.01	0.42
2:H:255:MET:HE1	2:H:399:LEU:HD13	2.01	0.42
1:G:161:SER:O	1:G:162:GLU:CB	2.68	0.42
2:H:288:HIS:CG	2:H:299:THR:HG22	2.55	0.42
2:F:54:GLN:O	2:F:58:VAL:HG23	2.20	0.42
2:F:221:PHE:O	2:F:225:VAL:HG23	2.19	0.42
2:D:133:TRP:CE3	2:D:134:LYS:HB2	2.55	0.41
2:B:106:VAL:O	2:B:109:THR:HG22	2.20	0.41
2:B:301:VAL:HG13	2:B:301:VAL:O	2.20	0.41
2:D:34:PHE:CZ	2:D:191:VAL:HG21	2.55	0.41
2:D:16:SER:C	2:D:17:THR:OG1	2.58	0.41
2:F:131:VAL:HG12	2:F:132:PRO:HB3	1.91	0.41
1:E:299:PRO:HG2	2:F:13:HIS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:THR:HG21	2:F:5:ILE:HG22	1.92	0.41
2:H:3:VAL:C	2:H:4:TYR:CG	2.92	0.41
1:G:217:LEU:CD1	1:G:219:ASP:HB2	2.47	0.41
2:D:144:ALA:O	2:D:148:LEU:HD12	2.19	0.41
2:B:148:LEU:HD22	2:B:197:TYR:HB2	2.01	0.41
2:B:255:MET:HE3	2:B:399:LEU:HB3	2.00	0.41
2:D:288:HIS:CG	2:D:299:THR:HG22	2.55	0.41
2:B:34:PHE:CZ	2:B:191:VAL:HG21	2.55	0.41
1:C:51:THR:CG2	2:D:83:ARG:NH1	2.65	0.41
2:D:135:ASP:C	2:D:136:LYS:HG3	2.40	0.41
2:B:131:VAL:HG12	2:B:132:PRO:HD3	1.99	0.41
2:D:72:MET:O	2:D:76:LEU:HD23	2.19	0.41
1:C:70:ASN:ND2	1:C:102:MET:HE3	2.34	0.41
2:H:255:MET:CE	2:H:399:LEU:HD13	2.50	0.41
2:F:175:VAL:HG12	2:F:200:VAL:HB	2.01	0.41
2:F:288:HIS:CG	2:F:299:THR:HG22	2.55	0.41
2:D:305:GLU:O	2:D:306:SER:C	2.59	0.41
2:F:201:VAL:HG12	2:F:203:PRO:HD3	2.01	0.41
2:F:206:LEU:HD21	2:F:214:ALA:HB1	2.03	0.41
1:E:165:LEU:HD23	1:E:165:LEU:N	2.35	0.41
2:B:14:ASN:ND2	2:B:14:ASN:N	2.65	0.41
2:F:133:TRP:CE3	2:F:134:LYS:HB2	2.55	0.41
2:D:93:GLY:O	2:D:95:VAL:HG23	2.21	0.41
1:C:161:SER:O	1:C:162:GLU:CB	2.68	0.41
1:E:161:SER:O	1:E:162:GLU:CB	2.68	0.41
2:D:34:PHE:CZ	2:D:186:LEU:HD11	2.56	0.41
2:D:142:LEU:O	2:D:146:LYS:CB	2.64	0.41
1:G:110:PRO:HA	2:H:131:VAL:O	2.19	0.41
2:F:144:ALA:O	2:F:148:LEU:CD1	2.69	0.41
2:B:48:GLU:HG2	2:B:171:LEU:HD11	2.01	0.41
2:B:305:GLU:O	2:B:306:SER:C	2.59	0.41
2:D:206:LEU:HD21	2:D:214:ALA:HB1	2.03	0.41
2:B:206:LEU:HD21	2:B:214:ALA:HB1	2.03	0.41
2:D:17:THR:HB	2:D:18:CYS:H	1.75	0.41
2:H:133:TRP:CE3	2:H:134:LYS:HB2	2.55	0.41
2:F:16:SER:C	2:F:17:THR:OG1	2.58	0.41
2:D:4:TYR:CE1	2:D:5:ILE:HD12	2.55	0.41
2:B:144:ALA:O	2:B:148:LEU:CD1	2.69	0.41
1:C:224:TYR:CE2	1:C:294:HIS:CE1	3.06	0.41
2:F:34:PHE:CZ	2:F:186:LEU:HD11	2.56	0.41
2:B:93:GLY:O	2:B:95:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:LEU:N	1:G:165:LEU:HD23	2.35	0.41
2:H:144:ALA:O	2:H:148:LEU:CD1	2.69	0.41
1:E:278:VAL:HG21	1:E:280:GLN:NE2	2.35	0.41
1:G:278:VAL:HG21	1:G:280:GLN:NE2	2.35	0.41
2:D:301:VAL:HG13	2:D:301:VAL:O	2.20	0.41
2:F:301:VAL:HG13	2:F:301:VAL:O	2.20	0.41
2:H:135:ASP:C	2:H:136:LYS:HG3	2.40	0.41
2:F:135:ASP:C	2:F:136:LYS:HG3	2.40	0.41
1:E:97:ILE:CA	2:H:449:LEU:HD22	2.50	0.41
1:A:224:TYR:CE2	1:A:294:HIS:CE1	3.06	0.41
1:A:278:VAL:HG21	1:A:280:GLN:NE2	2.35	0.41
1:A:161:SER:O	1:A:162:GLU:CB	2.68	0.41
2:F:279:MET:HB3	2:F:279:MET:HE3	1.90	0.41
1:C:165:LEU:N	1:C:165:LEU:HD23	2.35	0.41
2:D:69:ARG:NH1	2:D:133:TRP:HH2	2.13	0.41
2:B:133:TRP:CE3	2:B:134:LYS:HB2	2.55	0.41
2:H:4:TYR:CE1	2:H:5:ILE:HD12	2.55	0.41
2:H:93:GLY:O	2:H:95:VAL:HG23	2.21	0.41
2:F:98:ALA:HB2	2:F:353:LEU:HB3	2.03	0.41
1:G:74:LEU:HD12	1:G:76:LEU:HD11	2.03	0.41
2:D:98:ALA:HB2	2:D:353:LEU:HB3	2.03	0.41
1:C:210:CYS:O	1:C:210:CYS:SG	2.79	0.41
1:G:49:LEU:CB	2:H:127:ALA:HB1	2.48	0.41
2:D:255:MET:CE	2:D:399:LEU:HD13	2.50	0.41
2:D:48:GLU:HG2	2:D:171:LEU:HD11	2.01	0.41
2:H:305:GLU:O	2:H:306:SER:C	2.59	0.41
1:G:33:ASP:OD1	2:H:10:LEU:HB3	2.20	0.41
1:G:210:CYS:O	1:G:210:CYS:SG	2.79	0.41
2:H:132:PRO:HG2	2:H:135:ASP:C	2.40	0.40
2:B:135:ASP:C	2:B:136:LYS:HG3	2.40	0.40
2:F:176:VAL:CG2	2:F:198:THR:HG21	2.46	0.40
2:H:34:PHE:CZ	2:H:186:LEU:HD11	2.56	0.40
2:F:113:LEU:HD11	2:F:391:VAL:HG21	2.04	0.40
1:A:165:LEU:HD23	1:A:165:LEU:N	2.35	0.40
1:C:51:THR:HG21	2:D:83:ARG:NH1	2.34	0.40
2:H:142:LEU:O	2:H:146:LYS:CB	2.64	0.40
1:E:97:ILE:CA	2:H:449:LEU:CD2	2.97	0.40
2:H:3:VAL:HB	2:H:4:TYR:CG	2.43	0.40
1:E:49:LEU:HB3	2:F:128:ILE:N	2.36	0.40
1:A:207:THR:O	1:A:207:THR:HG22	2.21	0.40
2:D:144:ALA:O	2:D:148:LEU:CD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:VAL:O	2:F:109:THR:HG22	2.20	0.40
2:D:106:VAL:HG13	2:D:359:LEU:CD1	2.48	0.40
2:H:98:ALA:HB2	2:H:353:LEU:HB3	2.03	0.40
2:B:98:ALA:HB2	2:B:353:LEU:HB3	2.03	0.40
2:B:4:TYR:CE1	2:B:5:ILE:HD12	2.55	0.40
2:D:137:ASN:C	2:D:139:THR:H	2.25	0.40
1:G:224:TYR:HD2	1:G:294:HIS:CD2	2.33	0.40
1:G:206:SER:O	1:G:208:LEU:N	2.50	0.40
2:B:69:ARG:NH1	2:B:133:TRP:HH2	2.13	0.40
1:C:206:SER:O	1:C:208:LEU:N	2.50	0.40
2:B:255:MET:CE	2:B:399:LEU:HD22	2.52	0.40
1:G:251:LYS:HZ1	1:G:285:SER:HB2	1.83	0.40
2:B:34:PHE:CZ	2:B:186:LEU:HD11	2.56	0.40
1:A:48:ARG:HA	1:A:48:ARG:HD3	1.76	0.40
1:G:207:THR:HG22	1:G:207:THR:O	2.21	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:NE2	2:F:40:GLN:C[8_434]	0.58	1.62
2:B:40:GLN:C	2:F:40:GLN:NE2[8_434]	0.62	1.58
2:B:40:GLN:CA	2:F:40:GLN:NE2[8_434]	1.08	1.12
2:B:40:GLN:CD	2:F:40:GLN:C[8_434]	1.11	1.09
2:B:40:GLN:NE2	2:F:40:GLN:O[8_434]	1.14	1.06
2:B:40:GLN:C	2:F:40:GLN:CD[8_434]	1.15	1.05
2:B:40:GLN:NE2	2:F:40:GLN:CA[8_434]	1.29	0.91
2:B:40:GLN:O	2:F:40:GLN:NE2[8_434]	1.36	0.84
2:B:40:GLN:CG	2:F:40:GLN:CG[8_434]	1.37	0.83
2:B:40:GLN:OE1	2:F:41:ALA:N[8_434]	1.41	0.79
2:B:41:ALA:N	2:F:40:GLN:OE1[8_434]	1.44	0.76
1:A:23:THR:CG2	2:B:95:VAL:CG2[2_545]	1.51	0.69
1:C:257:THR:OG1	2:F:403:GLU:O[3_655]	1.59	0.61
2:B:40:GLN:CA	2:F:40:GLN:CD[8_434]	1.62	0.58
1:A:23:THR:CG2	2:B:95:VAL:CB[2_545]	1.62	0.58
2:B:40:GLN:CD	2:F:40:GLN:CA[8_434]	1.72	0.48
2:B:40:GLN:CD	2:F:40:GLN:O[8_434]	1.75	0.45
2:B:41:ALA:N	2:F:40:GLN:CD[8_434]	1.75	0.45
2:B:40:GLN:CB	2:F:40:GLN:CD[8_434]	1.78	0.42
2:B:40:GLN:CD	2:F:41:ALA:N[8_434]	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:OE1	2:F:40:GLN:C[8_434]	1.79	0.41
1:C:257:THR:CB	2:F:403:GLU:O[3_655]	1.86	0.34
2:B:40:GLN:C	2:F:40:GLN:OE1[8_434]	1.87	0.33
2:B:40:GLN:CB	2:F:40:GLN:CG[8_434]	1.88	0.32
2:B:40:GLN:CD	2:F:40:GLN:CB[8_434]	1.89	0.31
2:B:41:ALA:N	2:F:40:GLN:NE2[8_434]	1.89	0.31
2:B:40:GLN:NE2	2:F:41:ALA:N[8_434]	1.90	0.30
2:B:40:GLN:O	2:F:40:GLN:CD[8_434]	1.91	0.29
1:A:98:THR:N	2:B:449:LEU:CD2[2_545]	1.92	0.28
2:B:40:GLN:CG	2:F:40:GLN:CB[8_434]	2.00	0.20

5.3 Torsion angles

5.3.1 Protein backbone

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	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	46	83
1	C	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	46	83
1	E	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	46	83
1	G	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	46	83
2	B	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	7	49
2	D	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	7	49
2	F	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	7	49
2	H	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	7	49
All	All	2972/3340 (89%)	2692 (91%)	236 (8%)	44 (2%)	13	58

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	SER
2	B	15	GLU

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Mol	Chain	Res	Type
2	B	17	THR
1	C	206	SER
2	D	15	GLU
2	D	17	THR
1	E	206	SER
2	F	15	GLU
2	F	17	THR
1	G	206	SER
2	H	15	GLU
2	H	17	THR
2	B	4	TYR
2	B	139	THR
2	D	4	TYR
2	D	139	THR
2	F	4	TYR
2	F	139	THR
2	H	4	TYR
2	H	139	THR
2	B	144	ALA
2	B	379	GLN
2	D	144	ALA
2	D	379	GLN
2	F	144	ALA
2	F	379	GLN
2	H	144	ALA
2	H	379	GLN
2	B	295	ASN
2	B	437	THR
2	D	295	ASN
2	D	437	THR
2	F	295	ASN
2	F	437	THR
2	H	295	ASN
2	H	437	THR
2	B	336	MET
2	D	336	MET
2	F	336	MET
2	H	336	MET
2	B	352	VAL
2	D	352	VAL
2	F	352	VAL
2	H	352	VAL

5.3.2 Protein sidechains ⓘ

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	279/330 (84%)	265 (95%)	14 (5%)	30	68
1	C	279/330 (84%)	265 (95%)	14 (5%)	30	68
1	E	279/330 (84%)	265 (95%)	14 (5%)	30	68
1	G	279/330 (84%)	265 (95%)	14 (5%)	30	68
2	B	358/385 (93%)	340 (95%)	18 (5%)	30	68
2	D	358/385 (93%)	340 (95%)	18 (5%)	30	68
2	F	358/385 (93%)	340 (95%)	18 (5%)	30	68
2	H	358/385 (93%)	340 (95%)	18 (5%)	30	68
All	All	2548/2860 (89%)	2420 (95%)	128 (5%)	30	68

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	76	LEU
1	A	113	PRO
1	A	149	LYS
1	A	151	ASP
1	A	158	ASN
1	A	159	ARG
1	A	171	LEU
1	A	182	ASN
1	A	245	LEU
1	A	250	VAL
1	A	278	VAL
1	A	326	ARG
1	A	331	LEU
2	B	4	TYR
2	B	14	ASN
2	B	16	SER
2	B	17	THR
2	B	18	CYS

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Mol	Chain	Res	Type
2	B	54	GLN
2	B	101	LEU
2	B	118	LEU
2	B	204	ARG
2	B	266	GLU
2	B	296	PHE
2	B	333	LEU
2	B	347	THR
2	B	354	GLN
2	B	368	LEU
2	B	386	ILE
2	B	417	GLU
2	B	439	LEU
1	C	9	ASN
1	C	76	LEU
1	C	113	PRO
1	C	149	LYS
1	C	151	ASP
1	C	158	ASN
1	C	159	ARG
1	C	171	LEU
1	C	182	ASN
1	C	245	LEU
1	C	250	VAL
1	C	278	VAL
1	C	326	ARG
1	C	331	LEU
2	D	4	TYR
2	D	14	ASN
2	D	16	SER
2	D	17	THR
2	D	18	CYS
2	D	54	GLN
2	D	101	LEU
2	D	118	LEU
2	D	204	ARG
2	D	266	GLU
2	D	296	PHE
2	D	333	LEU
2	D	347	THR
2	D	354	GLN
2	D	368	LEU

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Mol	Chain	Res	Type
2	D	386	ILE
2	D	417	GLU
2	D	439	LEU
1	E	9	ASN
1	E	76	LEU
1	E	113	PRO
1	E	149	LYS
1	E	151	ASP
1	E	158	ASN
1	E	159	ARG
1	E	171	LEU
1	E	182	ASN
1	E	245	LEU
1	E	250	VAL
1	E	278	VAL
1	E	326	ARG
1	E	331	LEU
2	F	4	TYR
2	F	14	ASN
2	F	16	SER
2	F	17	THR
2	F	18	CYS
2	F	54	GLN
2	F	101	LEU
2	F	118	LEU
2	F	204	ARG
2	F	266	GLU
2	F	296	PHE
2	F	333	LEU
2	F	347	THR
2	F	354	GLN
2	F	368	LEU
2	F	386	ILE
2	F	417	GLU
2	F	439	LEU
1	G	9	ASN
1	G	76	LEU
1	G	113	PRO
1	G	149	LYS
1	G	151	ASP
1	G	158	ASN
1	G	159	ARG

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Mol	Chain	Res	Type
1	G	171	LEU
1	G	182	ASN
1	G	245	LEU
1	G	250	VAL
1	G	278	VAL
1	G	326	ARG
1	G	331	LEU
2	H	4	TYR
2	H	14	ASN
2	H	16	SER
2	H	17	THR
2	H	18	CYS
2	H	54	GLN
2	H	101	LEU
2	H	118	LEU
2	H	204	ARG
2	H	266	GLU
2	H	296	PHE
2	H	333	LEU
2	H	347	THR
2	H	354	GLN
2	H	368	LEU
2	H	386	ILE
2	H	417	GLU
2	H	439	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	101	GLN
1	A	141	ASN
1	A	158	ASN
1	A	195	GLN
1	A	197	GLN
1	A	264	HIS
1	A	280	GLN
2	B	13	HIS
2	B	14	ASN
2	B	137	ASN
2	B	188	GLN

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Mol	Chain	Res	Type
1	C	9	ASN
1	C	26	GLN
1	C	101	GLN
1	C	141	ASN
1	C	158	ASN
1	C	195	GLN
1	C	197	GLN
1	C	264	HIS
1	C	280	GLN
2	D	13	HIS
2	D	14	ASN
2	D	137	ASN
2	D	188	GLN
1	E	9	ASN
1	E	26	GLN
1	E	101	GLN
1	E	141	ASN
1	E	158	ASN
1	E	195	GLN
1	E	197	GLN
1	E	264	HIS
1	E	280	GLN
2	F	13	HIS
2	F	14	ASN
2	F	137	ASN
2	F	188	GLN
2	F	447	ASN
1	G	9	ASN
1	G	26	GLN
1	G	101	GLN
1	G	141	ASN
1	G	158	ASN
1	G	195	GLN
1	G	197	GLN
1	G	264	HIS
1	G	280	GLN
2	H	13	HIS
2	H	14	ASN
2	H	137	ASN
2	H	192	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/383 (86%)	0.67	35 (10%) 8 7	177, 273, 376, 684	0
1	C	330/383 (86%)	0.82	57 (17%) 2 3	200, 315, 406, 568	0
1	E	330/383 (86%)	0.81	56 (16%) 2 3	236, 314, 400, 518	0
1	G	330/383 (86%)	0.88	53 (16%) 3 4	240, 337, 443, 633	0
2	B	423/452 (93%)	1.22	82 (19%) 1 3	131, 273, 412, 537	1 (0%)
2	D	423/452 (93%)	1.68	143 (33%) 0 1	225, 360, 512, 725	1 (0%)
2	F	423/452 (93%)	1.25	91 (21%) 1 2	180, 285, 429, 757	1 (0%)
2	H	423/452 (93%)	1.74	143 (33%) 0 1	212, 357, 521, 686	1 (0%)
All	All	3012/3340 (90%)	1.18	660 (21%) 1 2	131, 317, 467, 757	4 (0%)

All (660) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	416	PRO	14.2
2	D	133	TRP	13.9
2	D	231	GLY	13.8
2	H	416	PRO	13.5
2	H	221	PHE	13.1
2	F	168	ALA	13.0
2	F	167	GLN	12.3
2	F	166	SER	12.3
1	G	95	GLY	12.2
2	B	417	GLU	11.9
1	G	134	ARG	10.9
2	H	133	TRP	10.8
2	H	233	SER	10.4
2	H	166	SER	10.4
2	F	447	ASN	10.2
2	H	167	GLN	10.1

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Mol	Chain	Res	Type	RSRZ
2	B	167	GLN	10.0
2	H	373	HIS	9.7
1	G	133	GLY	9.5
2	D	230	THR	9.5
2	B	403	GLU	9.5
1	G	96	GLY	9.4
2	H	168	ALA	9.3
2	D	337	LYS	9.1
2	D	132	PRO	9.1
2	B	133	TRP	8.5
2	H	370	ALA	8.5
2	H	417	GLU	8.4
2	D	134	LYS	8.3
2	F	449	LEU	8.3
2	F	133	TRP	8.2
2	F	446	ALA	8.1
2	F	337	LYS	8.1
2	D	44	SER	8.1
2	H	447	ASN	8.0
1	C	269	GLU	8.0
2	H	179	PHE	7.8
2	D	226	THR	7.7
2	H	301	VAL	7.7
2	F	416	PRO	7.6
2	H	218	ILE	7.6
2	D	416	PRO	7.6
2	F	334	ASN	7.1
2	D	386	ILE	7.1
2	B	140	SER	7.1
2	D	202	LEU	7.0
2	D	339	LEU	7.0
1	G	218	VAL	6.9
2	H	339	LEU	6.9
2	H	232	CYS	6.9
2	D	114	TYR	6.9
2	H	222	MET	6.9
1	E	182	ASN	6.8
2	D	367	GLU	6.8
2	F	448	PRO	6.8
2	D	43	THR	6.7
2	H	243	LEU	6.7
2	D	168	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
2	H	18	CYS	6.7
2	D	203	PRO	6.7
2	D	334	ASN	6.7
2	D	167	GLN	6.6
1	C	268	LYS	6.6
2	H	169	GLN	6.5
2	B	168	ALA	6.5
2	F	403	GLU	6.5
2	H	234	LEU	6.5
2	H	172	LEU	6.4
2	H	217	LYS	6.3
2	B	447	ASN	6.2
2	H	170	LEU	6.1
2	H	178	VAL	6.1
2	H	43	THR	6.1
2	H	6	HIS	6.1
1	G	172	GLY	6.1
2	D	3	VAL	6.0
2	B	374	THR	6.0
1	C	270	TYR	6.0
2	B	339	LEU	6.0
2	H	214	ALA	5.9
2	D	403	GLU	5.9
2	F	366	ALA	5.9
2	B	373	HIS	5.8
2	D	232	CYS	5.8
1	G	246	PHE	5.8
1	G	181	GLY	5.8
1	G	132	ILE	5.7
2	F	5	ILE	5.7
1	C	322	ARG	5.6
2	H	371	ILE	5.6
2	F	169	GLN	5.6
2	H	403	GLU	5.6
2	D	387	ARG	5.6
2	D	362	LEU	5.6
2	D	417	GLU	5.5
2	D	225	VAL	5.5
2	H	352	VAL	5.5
2	H	134	LYS	5.5
2	D	335	TRP	5.5
2	H	190	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	239	LEU	5.4
2	B	386	ILE	5.4
1	G	55	TYR	5.4
2	H	231	GLY	5.4
1	E	151	ASP	5.4
1	G	217	LEU	5.4
2	B	337	LYS	5.3
2	D	222	MET	5.3
2	B	141	ARG	5.2
2	H	386	ILE	5.2
2	F	164	ALA	5.2
2	H	337	LYS	5.2
1	E	266	GLY	5.2
2	D	172	LEU	5.2
2	H	164	ALA	5.1
2	H	174	THR	5.1
2	F	367	GLU	5.1
2	D	221	PHE	5.1
2	H	328	PHE	5.1
2	D	135	ASP	5.0
1	E	96	GLY	5.0
2	D	316	TYR	5.0
2	D	46	VAL	5.0
2	D	447	ASN	5.0
2	H	366	ALA	5.0
2	F	339	LEU	5.0
2	H	165	ASP	5.0
2	B	446	ALA	5.0
2	D	4	TYR	5.0
1	E	121	GLY	4.9
2	H	448	PRO	4.9
2	D	234	LEU	4.9
1	G	182	ASN	4.9
2	H	159	VAL	4.9
2	D	59	ALA	4.9
2	D	352	VAL	4.8
2	D	271	ASN	4.8
2	D	36	PRO	4.8
2	D	190	PHE	4.8
1	A	172	GLY	4.8
2	D	116	GLY	4.8
2	D	95	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	266	GLY	4.7
2	D	45	PRO	4.7
1	E	239	LEU	4.7
2	F	362	LEU	4.6
2	D	229	LYS	4.6
2	H	376	LEU	4.6
2	D	402	ASP	4.6
1	A	246	PHE	4.6
2	H	362	LEU	4.6
2	D	446	ALA	4.6
2	D	228	TRP	4.6
2	H	265	GLN	4.6
1	E	208	LEU	4.5
1	A	151	ASP	4.5
2	H	158	LEU	4.5
2	D	48	GLU	4.5
2	D	113	LEU	4.5
2	D	338	LYS	4.5
2	B	4	TYR	4.4
2	D	448	PRO	4.4
2	H	132	PRO	4.4
2	H	147	VAL	4.4
2	F	373	HIS	4.4
2	H	116	GLY	4.4
2	B	426	PRO	4.4
1	C	95	GLY	4.3
1	A	281	GLU	4.3
2	D	140	SER	4.3
1	E	80	THR	4.3
1	E	281	GLU	4.3
2	H	225	VAL	4.3
2	H	5	ILE	4.3
2	B	207	ASP	4.3
2	D	179	PHE	4.3
2	H	135	ASP	4.3
2	D	136	LYS	4.2
1	E	150	GLU	4.2
1	E	196	ILE	4.2
2	D	254	LYS	4.2
2	B	166	SER	4.2
1	E	118	GLU	4.2
2	D	245	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	285	THR	4.2
1	G	135	VAL	4.1
2	D	426	PRO	4.1
2	D	204	ARG	4.1
2	F	417	GLU	4.1
2	H	374	THR	4.1
2	B	402	ASP	4.1
2	H	209	THR	4.1
2	H	155	GLN	4.1
2	D	303	PHE	4.1
2	D	343	THR	4.1
1	C	58	LEU	4.0
2	D	353	LEU	4.0
2	D	5	ILE	4.0
1	C	96	GLY	4.0
1	C	21	ILE	4.0
2	B	367	GLU	4.0
1	C	203	VAL	4.0
2	H	264	PRO	4.0
2	B	427	PHE	4.0
2	H	312	ILE	4.0
1	E	327	ILE	4.0
1	G	208	LEU	4.0
2	D	186	LEU	3.9
2	H	338	LYS	3.9
1	G	308	LEU	3.9
2	H	369	PRO	3.9
1	G	94	VAL	3.9
2	H	334	ASN	3.9
2	F	386	ILE	3.9
1	G	245	LEU	3.9
2	H	139	THR	3.9
1	E	295	ALA	3.9
1	E	76	LEU	3.8
2	D	365	GLN	3.8
2	H	303	PHE	3.8
2	D	180	THR	3.8
1	C	298	ILE	3.8
2	B	370	ALA	3.8
1	E	329	PHE	3.8
2	F	287	GLN	3.8
2	B	387	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	H	300	GLN	3.7
2	H	160	ALA	3.7
1	E	181	GLY	3.7
1	A	270	TYR	3.7
1	C	235	LEU	3.7
1	A	302	THR	3.7
2	D	276	SER	3.7
2	F	352	VAL	3.7
2	H	55	LEU	3.7
2	H	256	LYS	3.7
1	G	116	LEU	3.7
2	F	255	MET	3.7
2	D	92	TRP	3.7
2	H	211	LEU	3.7
2	H	351	LEU	3.7
2	D	255	MET	3.6
2	H	399	LEU	3.6
2	D	349	PRO	3.6
2	D	237	ALA	3.6
1	E	267	GLY	3.5
1	E	135	VAL	3.5
1	E	265	LEU	3.5
2	H	194	LEU	3.5
1	G	80	THR	3.5
2	H	152	GLN	3.5
2	F	374	THR	3.5
2	H	202	LEU	3.5
1	E	134	ARG	3.5
1	C	246	PHE	3.5
2	H	363	LEU	3.5
1	A	286	LYS	3.5
1	E	206	SER	3.5
2	H	180	THR	3.5
2	B	352	VAL	3.5
2	H	8	PHE	3.5
1	E	268	LYS	3.5
1	C	155	PHE	3.5
2	H	220	ARG	3.4
1	C	271	THR	3.4
1	C	92	ILE	3.4
2	F	159	VAL	3.4
1	G	195	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	350	GLN	3.4
2	H	367	GLU	3.4
2	F	335	TRP	3.4
2	H	316	TYR	3.4
2	B	425	ARG	3.4
2	F	301	VAL	3.4
1	G	239	LEU	3.4
2	H	378	LEU	3.4
2	D	13	HIS	3.4
2	D	301	VAL	3.4
1	C	267	GLY	3.4
2	D	39	ILE	3.4
2	H	299	THR	3.4
2	D	284	GLY	3.4
2	F	238	SER	3.3
2	H	213	VAL	3.3
2	D	427	PHE	3.3
1	C	266	GLY	3.3
2	D	6	HIS	3.3
2	B	271	ASN	3.3
1	C	59	PHE	3.3
1	G	171	LEU	3.3
2	F	129	LEU	3.3
1	G	189	ILE	3.3
2	D	256	LYS	3.3
2	D	178	VAL	3.3
2	H	226	THR	3.3
2	F	385	ARG	3.3
2	B	313	GLN	3.3
2	H	95	VAL	3.2
1	G	197	GLN	3.2
2	F	351	LEU	3.2
2	H	390	GLU	3.2
2	H	215	ALA	3.2
2	B	362	LEU	3.2
2	B	162	GLY	3.2
2	F	445	VAL	3.2
1	E	83	VAL	3.2
2	B	312	ILE	3.2
1	C	42	PRO	3.2
2	F	294	ASP	3.2
2	H	137	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	203	PRO	3.2
1	A	132	ILE	3.2
1	G	191	THR	3.2
1	E	40	TRP	3.2
2	H	377	ASN	3.2
1	A	322	ARG	3.2
2	F	201	VAL	3.2
2	D	233	SER	3.2
1	G	243	LYS	3.2
2	D	397	PHE	3.2
1	G	148	LEU	3.1
1	G	193	VAL	3.1
2	H	52	GLN	3.1
1	E	165	LEU	3.1
1	G	203	VAL	3.1
2	B	338	LYS	3.1
2	F	254	LYS	3.1
2	B	327	THR	3.1
2	D	381	LEU	3.1
1	E	207	THR	3.1
2	D	206	LEU	3.1
2	D	261	LEU	3.1
2	D	201	VAL	3.1
1	G	32	PHE	3.1
2	F	444	ARG	3.1
2	F	286	PHE	3.1
2	B	444	ARG	3.1
1	A	148	LEU	3.1
2	D	171	LEU	3.1
2	D	166	SER	3.1
1	C	32	PHE	3.1
2	H	242	THR	3.1
2	H	92	TRP	3.1
2	F	91	LEU	3.0
1	E	32	PHE	3.0
2	F	178	VAL	3.0
1	C	184	HIS	3.0
1	C	182	ASN	3.0
1	C	57	LYS	3.0
2	H	171	LEU	3.0
1	A	150	GLU	3.0
1	G	97	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	16	SER	3.0
1	A	245	LEU	3.0
2	B	172	LEU	3.0
2	H	365	GLN	3.0
2	D	277	VAL	3.0
1	A	329	PHE	3.0
1	C	243	LYS	3.0
2	H	435	SER	3.0
1	C	162	GLU	3.0
2	B	83	ARG	3.0
2	B	399	LEU	3.0
1	C	171	LEU	3.0
2	D	357	TYR	3.0
1	A	171	LEU	2.9
2	D	218	ILE	2.9
2	F	170	LEU	2.9
2	B	5	ILE	2.9
2	H	173	SER	2.9
2	F	165	ASP	2.9
1	C	281	GLU	2.9
2	F	6	HIS	2.9
2	B	445	VAL	2.9
1	E	48	ARG	2.9
2	B	134	LYS	2.9
2	H	428	LEU	2.9
2	B	211	LEU	2.9
1	E	97	ILE	2.9
2	D	344	ILE	2.9
2	H	402	ASP	2.9
1	G	196	ILE	2.9
2	D	93	GLY	2.9
1	C	97	ILE	2.9
2	D	128	ILE	2.9
1	E	302	THR	2.9
2	H	244	ALA	2.8
2	H	204	ARG	2.8
2	B	43	THR	2.8
1	C	263	PHE	2.8
1	E	155	PHE	2.8
2	B	376	LEU	2.8
1	E	175	ASP	2.8
1	E	184	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	299	THR	2.8
1	G	13	THR	2.8
1	A	265	LEU	2.8
1	A	267	GLY	2.8
1	C	98	THR	2.8
2	D	445	VAL	2.8
2	F	388	VAL	2.8
1	A	155	PHE	2.8
1	C	133	GLY	2.8
1	G	214	CYS	2.8
2	D	336	MET	2.8
2	H	381	LEU	2.8
2	B	303	PHE	2.8
1	E	95	GLY	2.8
2	H	9	HIS	2.8
2	B	351	LEU	2.7
1	G	192	GLY	2.7
1	E	298	ILE	2.7
1	C	40	TRP	2.7
2	D	170	LEU	2.7
2	H	136	LYS	2.7
2	H	372	LEU	2.7
1	A	263	PHE	2.7
2	D	296	PHE	2.7
2	F	163	ARG	2.7
2	F	4	TYR	2.7
2	D	269	VAL	2.7
2	H	235	MET	2.7
1	E	133	GLY	2.7
1	C	91	ILE	2.7
2	H	186	LEU	2.7
2	H	425	ARG	2.7
1	E	186	ILE	2.7
2	D	354	GLN	2.6
2	F	399	LEU	2.6
2	D	143	ASP	2.6
2	D	211	LEU	2.6
2	F	202	LEU	2.6
2	H	388	VAL	2.6
2	D	183	GLY	2.6
1	A	219	ASP	2.6
2	B	202	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	402	ASP	2.6
2	B	87	MET	2.6
2	D	52	GLN	2.6
2	B	158	LEU	2.6
2	D	243	LEU	2.6
2	H	3	VAL	2.6
2	B	371	ILE	2.6
2	H	62	LEU	2.6
2	B	237	ALA	2.6
2	F	312	ILE	2.6
2	F	84	ILE	2.6
2	D	34	PHE	2.6
2	F	176	VAL	2.6
2	D	72	MET	2.6
2	F	67	LYS	2.6
2	D	84	ILE	2.6
1	G	156	TYR	2.6
1	E	116	LEU	2.5
1	C	145	GLN	2.5
2	B	3	VAL	2.5
2	F	338	LYS	2.5
2	D	331	ASN	2.5
2	D	449	LEU	2.5
1	A	287	LYS	2.5
2	H	67	LYS	2.5
2	D	182	PRO	2.5
2	F	426	PRO	2.5
2	F	376	LEU	2.5
2	F	52	GLN	2.5
2	F	303	PHE	2.5
2	H	255	MET	2.5
1	C	116	LEU	2.5
1	E	142	ILE	2.5
2	B	159	VAL	2.5
2	B	251	PHE	2.5
1	C	151	ASP	2.5
2	D	368	LEU	2.5
2	D	88	HIS	2.5
1	E	139	PHE	2.5
2	B	255	MET	2.5
1	E	201	VAL	2.5
2	B	170	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	293	GLN	2.5
1	G	157	TYR	2.5
2	F	363	LEU	2.5
1	G	19	ILE	2.5
2	H	395	ILE	2.5
2	H	296	PHE	2.5
2	F	300	GLN	2.4
2	H	84	ILE	2.4
1	C	69	HIS	2.4
1	A	125	MET	2.4
2	H	83	ARG	2.4
1	C	19	ILE	2.4
1	C	236	MET	2.4
1	C	41	VAL	2.4
2	D	235	MET	2.4
2	H	68	LEU	2.4
2	F	296	PHE	2.4
2	D	117	ALA	2.4
1	C	123	VAL	2.4
1	C	87	LEU	2.4
1	C	135	VAL	2.4
2	B	225	VAL	2.4
2	B	92	TRP	2.4
2	B	256	LYS	2.4
2	H	311	LEU	2.4
2	B	96	HIS	2.4
1	G	159	ARG	2.4
1	C	134	ARG	2.4
1	G	180	GLU	2.4
1	G	216	ALA	2.4
2	B	448	PRO	2.4
2	B	128	ILE	2.4
2	D	287	GLN	2.4
2	F	113	LEU	2.4
1	C	18	GLU	2.3
2	H	110	LEU	2.3
2	F	136	LYS	2.3
2	D	141	ARG	2.3
2	B	59	ALA	2.3
2	B	203	PRO	2.3
1	E	122	VAL	2.3
2	H	98	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	2.3
1	G	93	THR	2.3
2	H	51	LEU	2.3
2	H	287	GLN	2.3
1	G	199	LYS	2.3
2	F	59	ALA	2.3
1	A	272	LEU	2.3
1	C	105	GLU	2.3
1	E	132	ILE	2.3
2	F	155	GLN	2.3
2	F	349	PRO	2.3
2	D	363	LEU	2.3
2	H	210	GLU	2.3
1	A	55	TYR	2.3
1	G	18	GLU	2.3
2	B	169	GLN	2.3
2	F	162	GLY	2.3
2	F	313	GLN	2.3
1	E	13	THR	2.3
2	B	143	ASP	2.3
2	H	10	LEU	2.3
2	H	157	LEU	2.3
1	E	209	LEU	2.3
2	D	328	PHE	2.3
2	H	309	LEU	2.3
2	D	175	VAL	2.3
1	C	238	ALA	2.3
2	B	231	GLY	2.3
2	H	254	LYS	2.3
2	D	283	MET	2.3
2	D	356	SER	2.3
2	D	373	HIS	2.3
1	A	249	VAL	2.3
2	D	236	GLY	2.3
2	H	161	GLN	2.3
2	B	334	ASN	2.3
2	F	387	ARG	2.3
1	A	268	LYS	2.2
1	C	83	VAL	2.2
2	B	132	PRO	2.2
2	H	314	PRO	2.2
2	B	265	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	251	PHE	2.2
1	A	139	PHE	2.2
2	B	221	PHE	2.2
2	B	301	VAL	2.2
2	H	261	LEU	2.2
2	D	200	VAL	2.2
1	C	265	LEU	2.2
1	E	159	ARG	2.2
2	B	86	GLY	2.2
2	B	328	PHE	2.2
1	E	203	VAL	2.2
2	D	419	LEU	2.2
2	D	35	ILE	2.2
1	C	218	VAL	2.2
2	D	425	ARG	2.2
2	F	141	ARG	2.2
2	D	208	PHE	2.2
1	G	293	ILE	2.2
2	B	385	ARG	2.2
2	D	159	VAL	2.2
2	H	189	PRO	2.2
2	D	244	ALA	2.2
2	B	354	GLN	2.2
2	F	14	ASN	2.2
2	F	98	ALA	2.2
1	E	148	LEU	2.2
1	G	235	LEU	2.2
2	F	134	LYS	2.1
1	A	244	ARG	2.1
2	F	336	MET	2.1
1	E	331	LEU	2.1
2	H	113	LEU	2.1
2	H	206	LEU	2.1
2	D	139	THR	2.1
2	H	251	PHE	2.1
2	F	200	VAL	2.1
2	B	234	LEU	2.1
2	B	363	LEU	2.1
2	B	67	LYS	2.1
1	A	76	LEU	2.1
1	G	165	LEU	2.1
2	F	425	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	191	VAL	2.1
2	F	140	SER	2.1
2	F	291	ASP	2.1
2	H	327	THR	2.1
2	F	55	LEU	2.1
2	B	137	ASN	2.1
2	F	143	ASP	2.1
1	G	312	PHE	2.1
2	H	208	PHE	2.1
2	B	266	GLU	2.1
1	G	225	ILE	2.1
2	F	172	LEU	2.1
1	A	87	LEU	2.1
1	C	153	PHE	2.1
1	C	232	ILE	2.1
1	C	261	ILE	2.1
1	A	118	GLU	2.1
2	D	115	LEU	2.1
1	E	270	TYR	2.1
2	D	399	LEU	2.1
2	F	147	VAL	2.1
2	F	158	LEU	2.1
2	H	39	ILE	2.1
2	D	129	LEU	2.1
2	F	199	PRO	2.1
2	F	221	PHE	2.1
1	C	147	VAL	2.1
1	E	77	ARG	2.1
2	H	317	ALA	2.1
1	A	279	PHE	2.1
1	A	312	PHE	2.1
1	E	283	TYR	2.1
2	B	208	PHE	2.1
1	A	239	LEU	2.1
1	G	92	ILE	2.1
1	G	302	THR	2.1
2	D	374	THR	2.1
1	G	219	ASP	2.0
2	H	427	PHE	2.0
2	F	132	PRO	2.0
2	D	9	HIS	2.0
2	F	179	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	260	LEU	2.0
1	A	153	PHE	2.0
1	E	218	VAL	2.0
1	G	329	PHE	2.0
1	C	240	GLY	2.0
2	B	369	PRO	2.0
2	F	128	ILE	2.0
2	H	94	VAL	2.0
1	E	128	ILE	2.0
1	E	119	PHE	2.0
2	H	228	TRP	2.0
2	H	58	VAL	2.0
2	D	110	LEU	2.0
2	H	387	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.