



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3IZG
EMDB ID: : EMD-1321
Title : Bacteriophage T7 prohead shell EM-derived atomic model
Authors : Ionel, A.; Velazquez-Muriel, J.A.; Agirrezabala, X.; Luque, D.; Cuervo, A.;
Caston, J.R.; Valpuesta, J.M.; Martin-Benito, J.; Carrascosa, J.L.
Deposited on : 2010-10-27
Resolution : 10.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

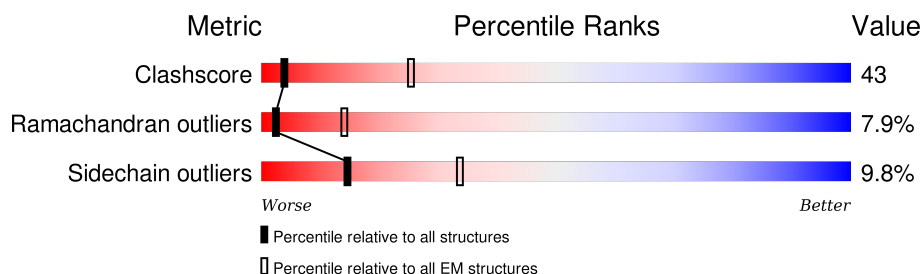
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
1	D	345	
1	E	345	
1	F	345	
1	G	345	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

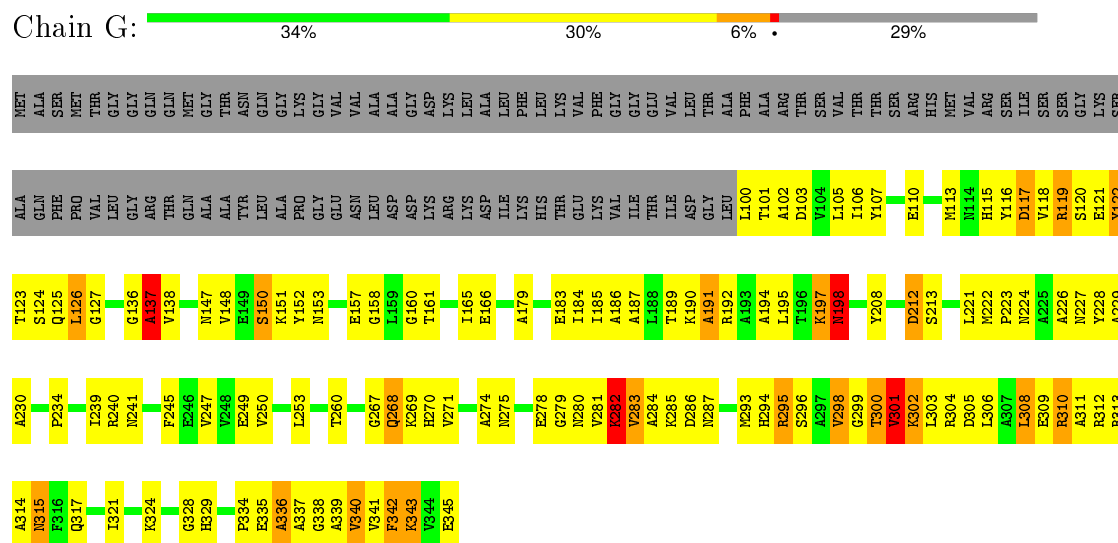
- Molecule 1 is a protein called Major capsid protein 10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	A	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	B	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	C	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	D	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	E	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		
1	F	246	Total	C	N	O	S	0	0
			1833	1147	321	357	8		

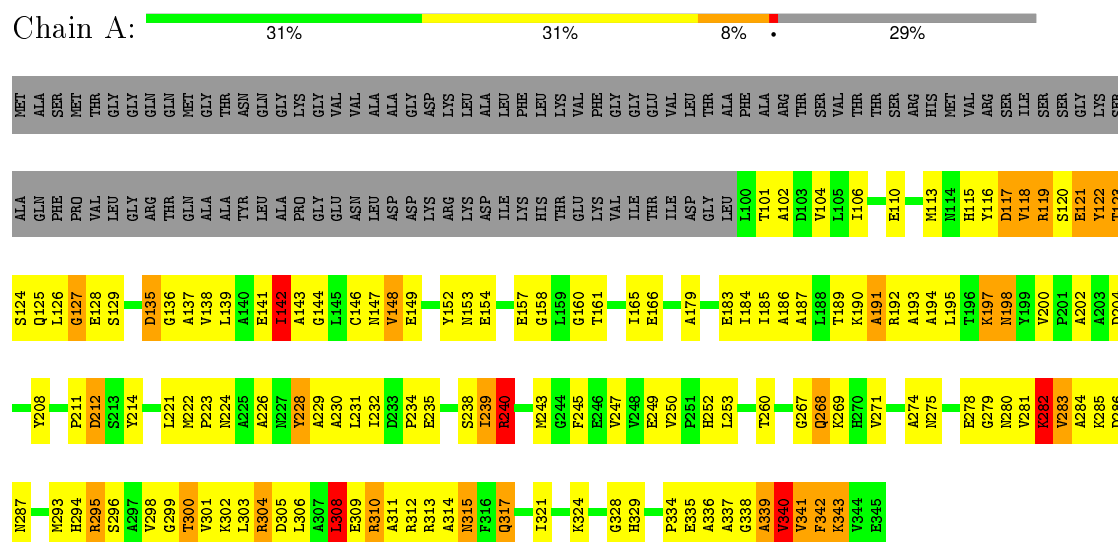
3 Residue-property plots

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. 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. 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.

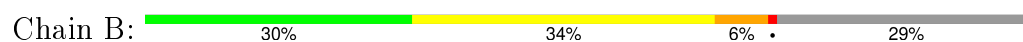
• Molecule 1: Major capsid protein 10A

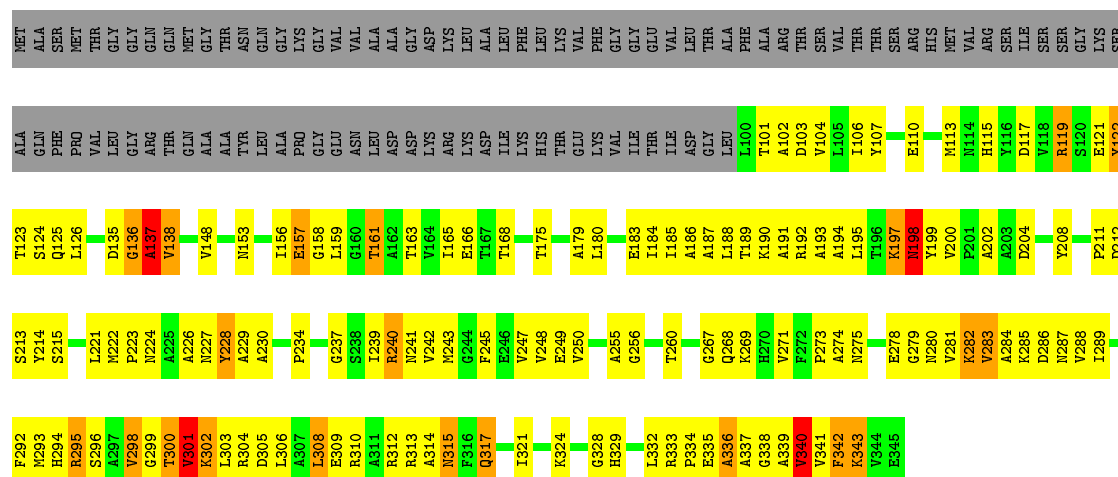


• Molecule 1: Major capsid protein 10A

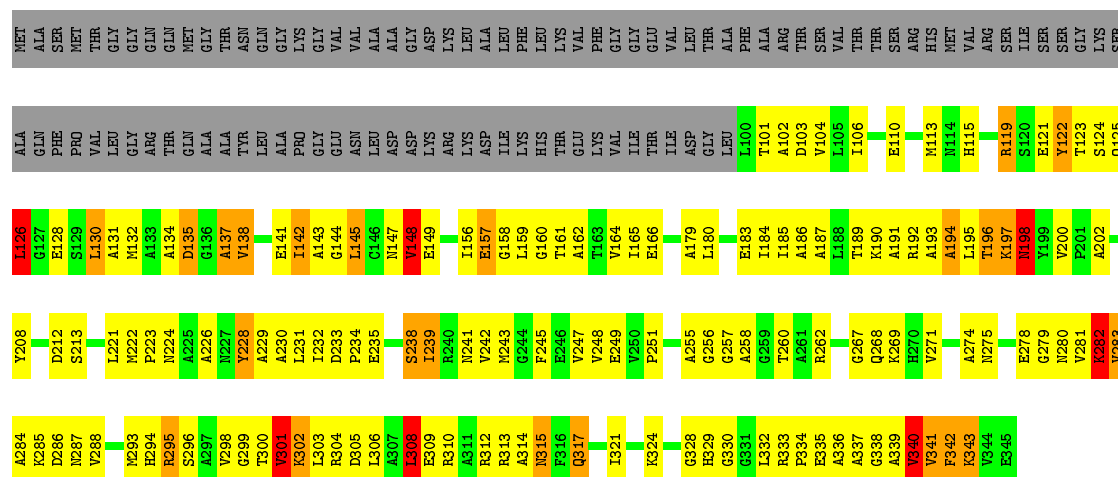
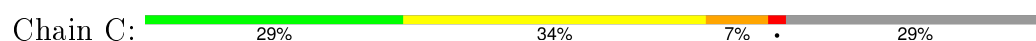


• Molecule 1: Major capsid protein 10A

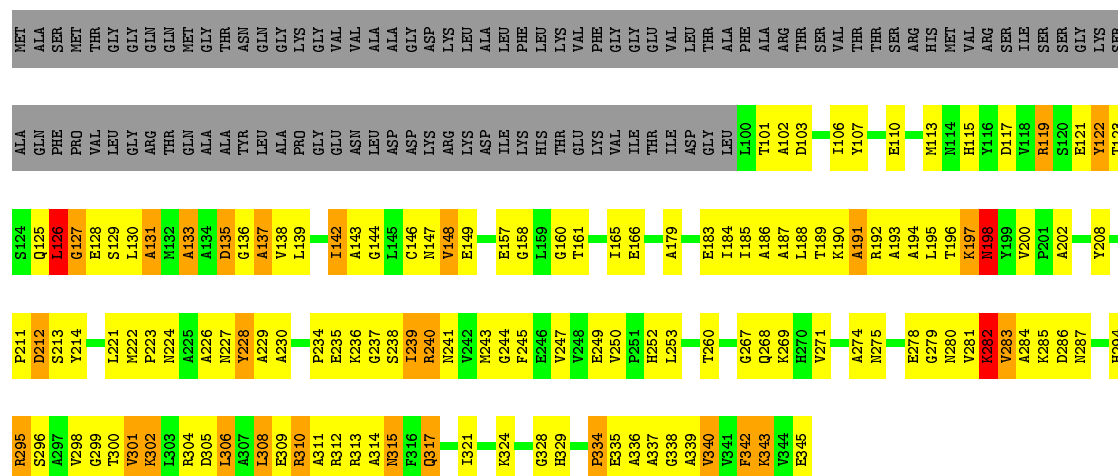




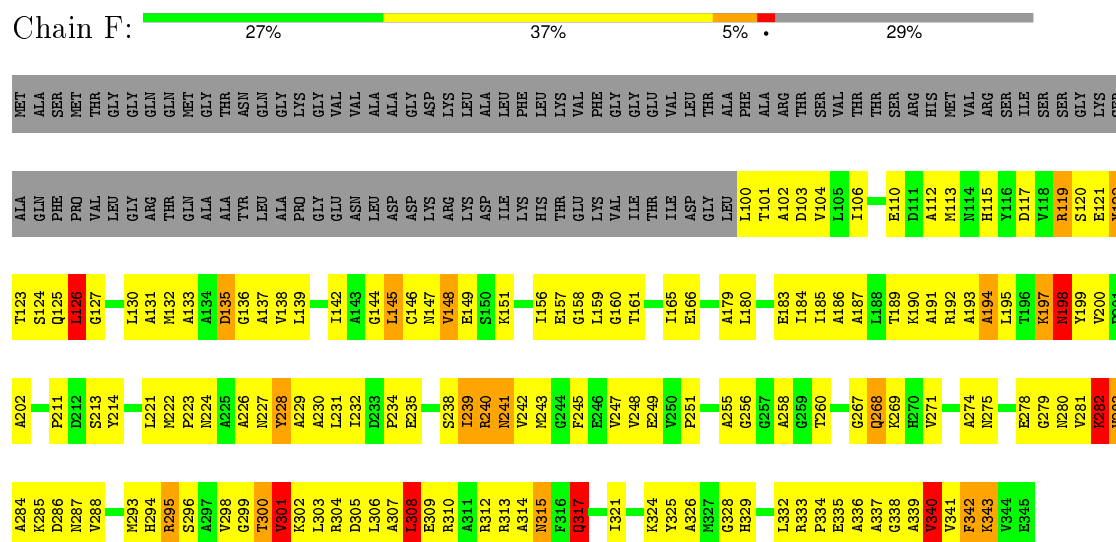
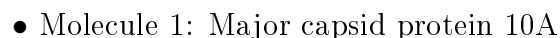
• Molecule 1: Major capsid protein 10A



• Molecule 1: Major capsid protein 10A



- Chain E: 33% 32% 5% • 29%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Wiener filter, defocus groups	Depositor
Microscope	Tecnai G2	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/1859	0.78	4/2518 (0.2%)
1	B	0.36	0/1859	0.97	4/2518 (0.2%)
1	C	0.43	1/1859 (0.1%)	0.99	7/2518 (0.3%)
1	D	0.35	0/1859	1.18	9/2518 (0.4%)
1	E	0.37	0/1859	1.14	6/2518 (0.2%)
1	F	0.36	0/1859	1.05	8/2518 (0.3%)
1	G	0.38	1/1859 (0.1%)	0.98	5/2518 (0.2%)
All	All	0.37	2/13013 (0.0%)	1.02	43/17626 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
1	G	0	4
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	301	VAL	C-O	10.12	1.42	1.23
1	G	301	VAL	C-O	5.44	1.33	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	GLN	CG-CD-OE1	-32.03	57.54	121.60
1	C	317	GLN	CG-CD-OE1	-31.99	57.62	121.60
1	G	317	GLN	CG-CD-OE1	-31.93	57.73	121.60
1	F	317	GLN	CG-CD-OE1	-30.51	60.58	121.60
1	D	317	GLN	CG-CD-OE1	-30.32	60.96	121.60
1	E	317	GLN	CG-CD-OE1	-30.14	61.32	121.60
1	D	301	VAL	CA-C-N	-21.84	69.16	117.20
1	E	301	VAL	CA-C-N	-21.70	69.47	117.20
1	D	301	VAL	O-C-N	-20.18	90.41	122.70
1	E	301	VAL	O-C-N	-19.73	91.14	122.70
1	A	317	GLN	CG-CD-OE1	-19.07	83.47	121.60
1	D	301	VAL	CA-C-O	18.74	159.45	120.10
1	E	301	VAL	CA-C-O	18.53	159.01	120.10
1	F	240	ARG	CA-C-N	-16.65	80.56	117.20
1	C	317	GLN	CG-CD-NE2	-14.81	81.15	116.70
1	B	317	GLN	CG-CD-NE2	-14.80	81.18	116.70
1	G	317	GLN	CG-CD-NE2	-14.79	81.19	116.70
1	F	317	GLN	CG-CD-NE2	-14.07	82.93	116.70
1	D	317	GLN	CG-CD-NE2	-14.01	83.08	116.70
1	F	240	ARG	O-C-N	13.99	145.09	122.70
1	E	317	GLN	CG-CD-NE2	-13.92	83.28	116.70
1	F	240	ARG	CA-C-O	-10.70	97.63	120.10
1	D	301	VAL	CA-CB-CG1	9.39	124.98	110.90
1	C	301	VAL	CA-C-N	-9.06	97.28	117.20
1	A	317	GLN	CG-CD-NE2	-8.68	95.87	116.70
1	G	301	VAL	N-CA-C	-8.60	87.77	111.00
1	B	301	VAL	N-CA-C	-7.68	90.27	111.00
1	B	317	GLN	OE1-CD-NE2	7.29	138.67	121.90
1	C	317	GLN	OE1-CD-NE2	7.29	138.66	121.90
1	G	317	GLN	OE1-CD-NE2	7.24	138.54	121.90
1	F	317	GLN	OE1-CD-NE2	7.17	138.39	121.90
1	E	317	GLN	OE1-CD-NE2	7.11	138.26	121.90
1	D	317	GLN	OE1-CD-NE2	7.11	138.25	121.90
1	C	301	VAL	N-CA-C	-6.37	93.81	111.00
1	A	301	VAL	N-CA-C	-6.12	94.49	111.00
1	F	301	VAL	N-CA-C	-5.99	94.82	111.00
1	D	301	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	C	301	VAL	CA-C-O	5.63	131.91	120.10
1	F	308	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	308	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	308	LEU	CA-CB-CG	5.19	127.23	115.30
1	G	301	VAL	CA-C-N	-5.00	106.19	117.20
1	D	138	VAL	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	THR	Peptide
1	A	317	GLN	Sidechain
1	B	136	GLY	Peptide
1	B	137	ALA	Peptide
1	B	300	THR	Peptide
1	C	137	ALA	Peptide
1	C	301	VAL	Mainchain
1	D	137	ALA	Peptide
1	D	317	GLN	Sidechain
1	E	317	GLN	Sidechain
1	F	240	ARG	Mainchain
1	F	300	THR	Peptide
1	F	317	GLN	Sidechain
1	G	136	GLY	Peptide
1	G	137	ALA	Peptide
1	G	300	THR	Peptide
1	G	301	VAL	Mainchain

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	1833	0	1832	185	0
1	B	1833	0	1832	165	0
1	C	1833	0	1832	177	0
1	D	1833	0	1831	145	0
1	E	1833	0	1830	157	0
1	F	1833	0	1832	164	0
1	G	1833	0	1832	184	0
All	All	12831	0	12821	1107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1107) 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:137:ALA:HB3	1:C:138:VAL:HB	1.20	1.11
1:B:137:ALA:HB1	1:B:138:VAL:HB	1.13	1.08
1:E:313:ARG:HD2	1:E:334:PRO:HB3	1.30	1.05
1:E:156:ILE:HB	1:F:135:ASP:HB3	1.36	1.04
1:B:313:ARG:HD2	1:B:334:PRO:HB3	1.39	1.04
1:F:313:ARG:HD2	1:F:334:PRO:HB3	1.38	1.04
1:G:122:TYR:CD1	1:G:306:LEU:HG	1.93	1.04
1:C:313:ARG:HD2	1:C:334:PRO:HB3	1.40	1.03
1:A:313:ARG:HD2	1:A:334:PRO:HB3	1.42	1.02
1:G:117:ASP:HB2	1:A:117:ASP:OD1	1.59	1.02
1:A:122:TYR:HB3	1:A:308:LEU:HB3	1.07	1.01
1:F:122:TYR:HB3	1:F:308:LEU:HB3	1.03	1.01
1:B:308:LEU:HD22	1:B:339:ALA:HB3	1.41	1.00
1:G:302:LYS:HG3	1:G:303:LEU:H	1.23	0.99
1:G:153:ASN:ND2	1:G:341:VAL:HG21	1.79	0.97
1:D:313:ARG:HD2	1:D:334:PRO:HB3	1.42	0.97
1:E:308:LEU:HD22	1:E:339:ALA:HB3	1.46	0.96
1:G:313:ARG:HD2	1:G:334:PRO:HB3	1.42	0.96
1:G:121:GLU:HG2	1:A:119:ARG:HH11	1.27	0.96
1:E:126:LEU:HA	1:E:302:LYS:HD2	1.47	0.96
1:G:119:ARG:CZ	1:A:152:TYR:HD2	1.77	0.96
1:C:159:LEU:HD13	1:D:135:ASP:HB3	1.49	0.95
1:D:126:LEU:HD22	1:D:127:GLY:H	1.29	0.95
1:B:126:LEU:HA	1:B:302:LYS:HD2	1.47	0.95
1:F:115:HIS:HB2	1:F:121:GLU:CB	1.99	0.93
1:C:122:TYR:CD1	1:C:306:LEU:HG	2.04	0.93
1:F:122:TYR:HB3	1:F:308:LEU:CB	1.96	0.92
1:B:122:TYR:CD1	1:B:306:LEU:HG	2.05	0.92
1:F:122:TYR:HD1	1:F:306:LEU:HG	1.34	0.91
1:G:308:LEU:HD22	1:G:339:ALA:HB3	1.51	0.91
1:F:122:TYR:CD1	1:F:306:LEU:HG	2.04	0.91
1:D:122:TYR:CD1	1:D:306:LEU:HG	2.05	0.91
1:A:152:TYR:O	1:A:153:ASN:ND2	2.04	0.91
1:C:137:ALA:CB	1:C:138:VAL:HB	2.00	0.91
1:D:301:VAL:H	1:D:302:LYS:HG3	1.32	0.91
1:D:308:LEU:HD22	1:D:339:ALA:HB3	1.53	0.90
1:D:301:VAL:H	1:D:302:LYS:CG	1.84	0.90
1:A:122:TYR:HD1	1:A:306:LEU:HG	1.34	0.90
1:E:122:TYR:CD1	1:E:306:LEU:HG	2.06	0.90
1:C:308:LEU:HD22	1:C:339:ALA:HB3	1.54	0.89
1:A:122:TYR:CD1	1:A:306:LEU:HG	2.07	0.89
1:C:115:HIS:HB2	1:C:121:GLU:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ALA:HA	1:G:340:VAL:HG21	1.55	0.89
1:A:117:ASP:HB2	1:A:119:ARG:HD3	1.53	0.88
1:B:137:ALA:CB	1:B:138:VAL:HB	2.02	0.87
1:G:119:ARG:NH2	1:A:152:TYR:HD2	1.71	0.87
1:A:195:LEU:HD23	1:A:341:VAL:H	1.40	0.87
1:A:126:LEU:HA	1:A:302:LYS:HB2	1.56	0.86
1:D:115:HIS:HB2	1:D:121:GLU:CB	2.05	0.86
1:A:117:ASP:CB	1:A:119:ARG:HD3	2.04	0.86
1:A:153:ASN:HD21	1:A:341:VAL:HG11	1.40	0.86
1:G:122:TYR:HD1	1:G:306:LEU:HG	1.42	0.85
1:B:191:ALA:HA	1:B:340:VAL:HG21	1.59	0.85
1:E:301:VAL:N	1:E:302:LYS:HG3	1.91	0.84
1:D:298:VAL:H	1:D:304:ARG:HH22	1.25	0.84
1:C:137:ALA:HB3	1:C:138:VAL:CB	2.05	0.84
1:F:115:HIS:HB2	1:F:121:GLU:HB3	1.57	0.84
1:G:245:PHE:CZ	1:G:300:THR:HG22	2.13	0.84
1:D:301:VAL:N	1:D:302:LYS:HG3	1.92	0.83
1:F:197:LYS:HA	1:F:342:PHE:CE2	2.14	0.83
1:G:116:TYR:O	1:A:116:TYR:O	1.97	0.83
1:D:306:LEU:HB3	1:D:343:LYS:HE3	1.61	0.83
1:A:120:SER:HB2	1:A:308:LEU:HD23	1.61	0.82
1:E:122:TYR:HD1	1:E:306:LEU:HG	1.42	0.82
1:B:273:PRO:HB3	1:C:282:LYS:HB3	1.61	0.82
1:D:191:ALA:HA	1:D:340:VAL:HG21	1.60	0.82
1:E:191:ALA:HA	1:E:340:VAL:HG21	1.62	0.82
1:E:161:THR:O	1:F:130:LEU:HD13	1.79	0.81
1:C:197:LYS:HA	1:C:342:PHE:CE2	2.16	0.81
1:C:115:HIS:HB2	1:C:121:GLU:HB2	1.62	0.81
1:A:191:ALA:HA	1:A:340:VAL:HG21	1.63	0.81
1:G:121:GLU:HG2	1:A:119:ARG:NH1	1.95	0.81
1:C:122:TYR:HD1	1:C:306:LEU:HG	1.42	0.81
1:E:224:ASN:HB2	1:E:260:THR:HG21	1.63	0.80
1:C:128:GLU:HB2	1:C:130:LEU:HD21	1.63	0.80
1:A:122:TYR:CB	1:A:308:LEU:HB3	2.02	0.80
1:G:191:ALA:HA	1:G:340:VAL:CG2	2.11	0.80
1:F:245:PHE:CZ	1:F:300:THR:HG22	2.17	0.80
1:F:224:ASN:HB2	1:F:260:THR:HG21	1.63	0.80
1:G:119:ARG:NH2	1:A:152:TYR:CD2	2.49	0.80
1:F:187:ALA:HA	1:F:190:LYS:HB2	1.64	0.80
1:F:306:LEU:HB3	1:F:343:LYS:HE3	1.65	0.79
1:B:194:ALA:HB3	1:B:340:VAL:CG2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:TYR:HD1	1:D:306:LEU:HG	1.47	0.79
1:B:156:ILE:H	1:C:135:ASP:HB3	1.45	0.79
1:A:197:LYS:HA	1:A:342:PHE:CE2	2.17	0.79
1:C:122:TYR:CG	1:C:308:LEU:HG	2.17	0.79
1:E:115:HIS:HB2	1:E:121:GLU:CB	2.13	0.79
1:A:120:SER:HB2	1:A:308:LEU:CD2	2.13	0.79
1:A:125:GLN:O	1:A:302:LYS:HD2	1.82	0.79
1:F:144:GLY:O	1:F:145:LEU:HB2	1.79	0.79
1:B:122:TYR:HD1	1:B:306:LEU:HG	1.46	0.78
1:B:224:ASN:HB2	1:B:260:THR:HG21	1.64	0.78
1:C:144:GLY:O	1:C:145:LEU:HB2	1.84	0.78
1:A:224:ASN:HB2	1:A:260:THR:HG21	1.64	0.78
1:G:127:GLY:N	1:G:302:LYS:HD2	1.99	0.78
1:E:278:GLU:HG3	1:E:285:LYS:HB3	1.65	0.78
1:F:122:TYR:CB	1:F:308:LEU:HB3	1.99	0.77
1:A:278:GLU:HG3	1:A:285:LYS:HB3	1.66	0.77
1:B:137:ALA:HB1	1:B:138:VAL:CB	2.05	0.77
1:F:120:SER:HB2	1:F:308:LEU:CD2	2.14	0.77
1:A:306:LEU:HB3	1:A:343:LYS:HE3	1.67	0.77
1:A:153:ASN:ND2	1:A:341:VAL:HG11	1.99	0.76
1:F:179:ALA:O	1:F:183:GLU:HG2	1.85	0.76
1:B:194:ALA:HB3	1:B:340:VAL:HG22	1.67	0.76
1:D:224:ASN:HB2	1:D:260:THR:HG21	1.65	0.76
1:G:224:ASN:HB2	1:G:260:THR:HG21	1.67	0.76
1:B:115:HIS:HB2	1:B:121:GLU:CB	2.16	0.76
1:B:278:GLU:HG3	1:B:285:LYS:HB3	1.67	0.76
1:D:278:GLU:HG3	1:D:285:LYS:HB3	1.68	0.76
1:D:187:ALA:HA	1:D:190:LYS:HB2	1.68	0.75
1:G:302:LYS:HG3	1:G:303:LEU:N	2.01	0.75
1:F:120:SER:HB2	1:F:308:LEU:HD21	1.67	0.75
1:D:198:ASN:H	1:D:342:PHE:HZ	1.35	0.75
1:A:194:ALA:HB3	1:A:340:VAL:CG2	2.17	0.75
1:C:198:ASN:H	1:C:342:PHE:HZ	1.33	0.75
1:E:179:ALA:O	1:E:183:GLU:HG2	1.86	0.75
1:G:278:GLU:HG3	1:G:285:LYS:HB3	1.67	0.75
1:E:194:ALA:HB3	1:E:340:VAL:CG2	2.16	0.75
1:C:278:GLU:HG3	1:C:285:LYS:HB3	1.68	0.75
1:D:115:HIS:HB2	1:D:121:GLU:HB2	1.69	0.75
1:A:314:ALA:HB2	1:A:337:ALA:HB2	1.69	0.75
1:C:224:ASN:HB2	1:C:260:THR:HG21	1.67	0.74
1:A:191:ALA:HA	1:A:340:VAL:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:PRO:HB3	1:F:282:LYS:HB3	1.69	0.74
1:D:194:ALA:HB3	1:D:340:VAL:CG2	2.17	0.74
1:B:179:ALA:O	1:B:183:GLU:HG2	1.86	0.74
1:G:117:ASP:OD1	1:A:117:ASP:HB2	1.87	0.74
1:G:195:LEU:HD23	1:G:341:VAL:H	1.51	0.74
1:E:161:THR:HG23	1:F:130:LEU:HB3	1.70	0.74
1:B:247:VAL:H	1:B:280:ASN:ND2	1.86	0.73
1:D:197:LYS:HA	1:D:342:PHE:CE2	2.23	0.73
1:C:191:ALA:HA	1:C:340:VAL:HG21	1.69	0.73
1:C:135:ASP:O	1:C:138:VAL:HG12	1.88	0.73
1:E:191:ALA:HA	1:E:340:VAL:CG2	2.18	0.73
1:C:179:ALA:O	1:C:183:GLU:HG2	1.88	0.73
1:B:247:VAL:H	1:B:280:ASN:HD22	1.37	0.73
1:F:278:GLU:HG3	1:F:285:LYS:HB3	1.71	0.73
1:D:191:ALA:HA	1:D:340:VAL:CG2	2.19	0.73
1:C:194:ALA:HB3	1:C:340:VAL:CG2	2.18	0.73
1:G:298:VAL:H	1:G:304:ARG:HH22	1.37	0.73
1:G:197:LYS:HA	1:G:342:PHE:CE2	2.24	0.73
1:G:115:HIS:CD2	1:G:121:GLU:HB3	2.24	0.73
1:C:187:ALA:HA	1:C:190:LYS:HB2	1.70	0.73
1:F:115:HIS:HB2	1:F:121:GLU:HB2	1.68	0.72
1:A:126:LEU:O	1:A:128:GLU:N	2.22	0.72
1:G:194:ALA:HB3	1:G:340:VAL:CG2	2.19	0.72
1:C:251:PRO:HB2	1:D:235:GLU:HG2	1.71	0.72
1:G:187:ALA:HA	1:G:190:LYS:HB2	1.70	0.72
1:C:235:GLU:O	1:C:238:SER:HB3	1.89	0.72
1:C:115:HIS:HB2	1:C:121:GLU:HB3	1.70	0.72
1:A:195:LEU:HG	1:A:340:VAL:HG23	1.72	0.71
1:G:194:ALA:HB3	1:G:340:VAL:HG22	1.72	0.71
1:A:179:ALA:O	1:A:183:GLU:HG2	1.90	0.71
1:G:121:GLU:CG	1:A:119:ARG:HH11	2.00	0.71
1:B:191:ALA:HA	1:B:340:VAL:CG2	2.19	0.71
1:G:179:ALA:O	1:G:183:GLU:HG2	1.91	0.71
1:C:308:LEU:HD12	1:C:308:LEU:H	1.54	0.71
1:E:187:ALA:HA	1:E:190:LYS:HB2	1.72	0.70
1:B:187:ALA:HA	1:B:190:LYS:HB2	1.72	0.70
1:A:235:GLU:HG2	1:F:251:PRO:HB2	1.72	0.70
1:C:194:ALA:HB3	1:C:340:VAL:HG21	1.73	0.70
1:G:137:ALA:CB	1:G:138:VAL:HB	2.20	0.70
1:A:119:ARG:HG2	1:A:120:SER:N	2.07	0.70
1:E:306:LEU:HB3	1:E:343:LYS:HE3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:ASN:H	1:G:342:PHE:HZ	1.40	0.69
1:D:194:ALA:HB3	1:D:340:VAL:HG22	1.72	0.69
1:G:137:ALA:HB1	1:G:138:VAL:HB	1.73	0.69
1:A:235:GLU:OE1	1:F:255:ALA:HB2	1.92	0.69
1:G:314:ALA:HB2	1:G:337:ALA:HB2	1.74	0.69
1:A:135:ASP:HB3	1:F:159:LEU:HD13	1.75	0.69
1:F:126:LEU:HA	1:F:302:LYS:HD2	1.75	0.69
1:B:241:ASN:OD1	1:B:300:THR:HG21	1.92	0.69
1:F:194:ALA:HB3	1:F:340:VAL:HG21	1.75	0.69
1:D:179:ALA:O	1:D:183:GLU:HG2	1.91	0.69
1:G:153:ASN:HD21	1:G:341:VAL:HG11	1.55	0.69
1:F:321:ILE:HB	1:F:324:LYS:HB2	1.75	0.69
1:G:117:ASP:OD2	1:A:115:HIS:HB2	1.92	0.69
1:G:117:ASP:HB2	1:A:119:ARG:CZ	2.23	0.69
1:A:142:ILE:C	1:A:144:GLY:H	1.96	0.68
1:A:187:ALA:HA	1:A:190:LYS:HB2	1.73	0.68
1:B:115:HIS:HB2	1:B:121:GLU:HB2	1.75	0.68
1:C:321:ILE:HB	1:C:324:LYS:HB2	1.75	0.68
1:G:115:HIS:HB3	1:A:118:VAL:H	1.58	0.68
1:F:138:VAL:HG22	1:F:139:LEU:H	1.59	0.68
1:A:298:VAL:H	1:A:304:ARG:HH22	1.39	0.68
1:F:234:PRO:HA	1:F:298:VAL:HG13	1.76	0.68
1:B:301:VAL:H	1:B:302:LYS:HG3	1.58	0.68
1:C:234:PRO:HA	1:C:298:VAL:HG13	1.76	0.68
1:C:247:VAL:H	1:C:280:ASN:ND2	1.92	0.68
1:A:321:ILE:HB	1:A:324:LYS:HB2	1.76	0.68
1:F:191:ALA:HA	1:F:340:VAL:HG21	1.75	0.68
1:E:122:TYR:HB3	1:E:308:LEU:HG	1.76	0.68
1:D:239:ILE:HG13	1:D:240:ARG:N	2.08	0.68
1:A:194:ALA:HB3	1:A:340:VAL:HG22	1.74	0.68
1:E:314:ALA:HB2	1:E:337:ALA:HB2	1.76	0.68
1:C:194:ALA:HA	1:C:342:PHE:CZ	2.29	0.68
1:B:315:ASN:HD22	1:B:315:ASN:H	1.40	0.67
1:A:119:ARG:HE	1:A:121:GLU:HG3	1.60	0.67
1:B:302:LYS:HE3	1:B:303:LEU:HB2	1.75	0.67
1:E:247:VAL:H	1:E:280:ASN:ND2	1.91	0.67
1:B:156:ILE:H	1:C:135:ASP:CB	2.07	0.67
1:D:122:TYR:CG	1:D:308:LEU:HG	2.29	0.67
1:G:115:HIS:HB2	1:A:117:ASP:OD2	1.94	0.67
1:E:247:VAL:H	1:E:280:ASN:HD22	1.43	0.67
1:F:119:ARG:HE	1:F:121:GLU:HG3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:HIS:HB2	1:D:121:GLU:HB3	1.76	0.67
1:A:222:MET:HB3	1:A:223:PRO:HD3	1.77	0.67
1:E:309:GLU:HA	1:E:338:GLY:HA3	1.77	0.67
1:G:222:MET:HB3	1:G:223:PRO:HD3	1.77	0.67
1:D:314:ALA:HB2	1:D:337:ALA:HB2	1.76	0.67
1:C:234:PRO:HB2	1:C:282:LYS:HD2	1.75	0.67
1:B:314:ALA:HB2	1:B:337:ALA:HB2	1.75	0.66
1:E:194:ALA:HB3	1:E:340:VAL:HG22	1.75	0.66
1:C:122:TYR:HB3	1:C:308:LEU:HG	1.77	0.66
1:D:222:MET:HB3	1:D:223:PRO:HD3	1.77	0.66
1:E:160:GLY:HA2	1:F:132:MET:HG2	1.77	0.66
1:C:222:MET:HB3	1:C:223:PRO:HD3	1.78	0.66
1:E:161:THR:HA	1:E:333:ARG:HA	1.77	0.66
1:B:300:THR:HA	1:B:301:VAL:HG13	1.78	0.66
1:D:245:PHE:CZ	1:D:300:THR:HG22	2.31	0.65
1:G:247:VAL:H	1:G:280:ASN:ND2	1.94	0.65
1:D:321:ILE:HB	1:D:324:LYS:HB2	1.78	0.65
1:B:309:GLU:HA	1:B:338:GLY:HA3	1.76	0.65
1:G:122:TYR:CG	1:G:308:LEU:HG	2.31	0.65
1:F:222:MET:HB3	1:F:223:PRO:HD3	1.77	0.65
1:A:117:ASP:OD1	1:A:119:ARG:CZ	2.45	0.65
1:G:195:LEU:HG	1:G:340:VAL:HG23	1.79	0.65
1:E:313:ARG:HD2	1:E:334:PRO:CB	2.18	0.65
1:C:269:LYS:HG2	1:C:281:VAL:HG13	1.79	0.64
1:A:269:LYS:HG2	1:A:281:VAL:HG13	1.80	0.64
1:G:125:GLN:HA	1:G:148:VAL:HA	1.79	0.64
1:B:122:TYR:CG	1:B:308:LEU:HG	2.32	0.64
1:A:102:ALA:HB3	1:A:189:THR:HB	1.80	0.64
1:G:117:ASP:N	1:A:117:ASP:OD1	2.31	0.64
1:A:126:LEU:HA	1:A:302:LYS:CB	2.27	0.64
1:F:235:GLU:O	1:F:238:SER:HB3	1.97	0.64
1:C:119:ARG:HE	1:C:121:GLU:HG3	1.63	0.64
1:E:102:ALA:HB3	1:E:189:THR:HB	1.79	0.64
1:G:110:GLU:CD	1:G:305:ASP:HB3	2.18	0.64
1:A:161:THR:HA	1:A:334:PRO:HD2	1.79	0.64
1:E:239:ILE:O	1:E:240:ARG:HG3	1.97	0.64
1:E:269:LYS:HG2	1:E:281:VAL:HG13	1.80	0.64
1:F:314:ALA:HB2	1:F:337:ALA:HB2	1.80	0.64
1:B:306:LEU:HB3	1:B:343:LYS:HE3	1.79	0.64
1:G:247:VAL:H	1:G:280:ASN:HD22	1.46	0.64
1:A:315:ASN:HD22	1:A:315:ASN:H	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:ASN:HD22	1:E:315:ASN:H	1.46	0.63
1:A:119:ARG:HH21	1:A:121:GLU:HG3	1.63	0.63
1:C:247:VAL:H	1:C:280:ASN:HD22	1.45	0.63
1:E:115:HIS:HB2	1:E:121:GLU:HB2	1.80	0.63
1:G:230:ALA:O	1:G:234:PRO:HD2	1.98	0.63
1:E:274:ALA:HA	1:E:287:ASN:HD22	1.62	0.63
1:C:126:LEU:HD23	1:C:302:LYS:HE3	1.81	0.63
1:A:106:ILE:HB	1:A:192:ARG:HB3	1.79	0.63
1:G:126:LEU:HA	1:G:302:LYS:CB	2.29	0.63
1:D:195:LEU:HG	1:D:340:VAL:HG23	1.79	0.63
1:E:122:TYR:CG	1:E:308:LEU:HG	2.34	0.63
1:C:197:LYS:HA	1:C:342:PHE:CZ	2.34	0.62
1:E:222:MET:HB3	1:E:223:PRO:HD3	1.81	0.62
1:B:274:ALA:HA	1:B:287:ASN:HD22	1.64	0.62
1:G:230:ALA:HA	1:G:296:SER:HB2	1.80	0.62
1:F:269:LYS:HG2	1:F:281:VAL:HG13	1.82	0.62
1:C:191:ALA:HA	1:C:340:VAL:CG2	2.30	0.62
1:G:301:VAL:H	1:G:302:LYS:HG2	1.65	0.62
1:G:124:SER:HB3	1:G:306:LEU:HB2	1.82	0.62
1:F:239:ILE:HG13	1:F:241:ASN:HB2	1.81	0.62
1:G:321:ILE:HB	1:G:324:LYS:HB2	1.79	0.62
1:F:306:LEU:CB	1:F:343:LYS:HE3	2.28	0.62
1:E:321:ILE:HB	1:E:324:LYS:HB2	1.82	0.61
1:B:269:LYS:HG2	1:B:281:VAL:HG13	1.80	0.61
1:C:309:GLU:HA	1:C:338:GLY:HA3	1.83	0.61
1:G:119:ARG:CZ	1:A:152:TYR:CD2	2.69	0.61
1:B:102:ALA:HB3	1:B:189:THR:HB	1.82	0.61
1:G:122:TYR:HB3	1:G:308:LEU:HG	1.81	0.61
1:D:247:VAL:H	1:D:280:ASN:ND2	1.99	0.61
1:A:106:ILE:O	1:A:110:GLU:HB2	2.01	0.61
1:B:115:HIS:NE2	1:B:123:THR:HG22	2.15	0.61
1:B:313:ARG:HD2	1:B:334:PRO:CB	2.24	0.61
1:C:306:LEU:HB3	1:C:343:LYS:HE3	1.82	0.61
1:D:315:ASN:H	1:D:315:ASN:HD22	1.49	0.61
1:B:312:ARG:O	1:B:337:ALA:HB3	2.01	0.61
1:A:153:ASN:ND2	1:A:341:VAL:HG21	2.16	0.61
1:E:126:LEU:CA	1:E:302:LYS:HD2	2.28	0.61
1:E:161:THR:HA	1:E:334:PRO:HD2	1.82	0.60
1:A:247:VAL:H	1:A:280:ASN:HD22	1.49	0.60
1:A:230:ALA:O	1:A:234:PRO:HD2	2.01	0.60
1:G:126:LEU:C	1:G:302:LYS:HD2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:PHE:CZ	1:E:300:THR:HG22	2.36	0.60
1:C:308:LEU:HD13	1:C:339:ALA:C	2.22	0.60
1:G:245:PHE:HZ	1:G:300:THR:HG22	1.65	0.60
1:F:125:GLN:HA	1:F:148:VAL:HG23	1.82	0.60
1:F:315:ASN:HD22	1:F:315:ASN:H	1.50	0.60
1:G:117:ASP:CB	1:A:117:ASP:OD1	2.42	0.60
1:E:301:VAL:N	1:E:302:LYS:CG	2.64	0.60
1:D:230:ALA:HA	1:D:296:SER:HB2	1.82	0.60
1:D:234:PRO:HA	1:D:298:VAL:HG13	1.83	0.60
1:B:222:MET:HB3	1:B:223:PRO:HD3	1.82	0.60
1:B:194:ALA:CB	1:B:340:VAL:HG22	2.31	0.60
1:D:115:HIS:NE2	1:D:123:THR:CG2	2.64	0.60
1:G:279:GLY:HA2	1:G:284:ALA:HA	1.84	0.60
1:A:247:VAL:H	1:A:280:ASN:ND2	1.99	0.60
1:A:235:GLU:CG	1:F:251:PRO:HB2	2.31	0.60
1:D:126:LEU:HA	1:D:302:LYS:HB2	1.83	0.60
1:C:306:LEU:CB	1:C:343:LYS:HE3	2.32	0.60
1:G:302:LYS:CG	1:G:303:LEU:H	1.93	0.59
1:B:237:GLY:HA2	1:B:241:ASN:HB3	1.83	0.59
1:D:247:VAL:H	1:D:280:ASN:HD22	1.50	0.59
1:B:283:VAL:HG22	1:B:284:ALA:H	1.67	0.59
1:F:230:ALA:HA	1:F:296:SER:HB2	1.84	0.59
1:F:194:ALA:HB3	1:F:340:VAL:CG2	2.32	0.59
1:C:308:LEU:CD2	1:C:339:ALA:HB3	2.29	0.59
1:E:313:ARG:HH21	1:E:334:PRO:HA	1.66	0.59
1:G:152:TYR:O	1:G:153:ASN:ND2	2.35	0.59
1:F:274:ALA:HA	1:F:287:ASN:HD22	1.68	0.59
1:A:136:GLY:HA2	1:F:156:ILE:HB	1.82	0.59
1:C:314:ALA:HB2	1:C:337:ALA:HB2	1.83	0.59
1:C:255:ALA:HB2	1:D:235:GLU:OE1	2.01	0.59
1:C:231:LEU:O	1:C:235:GLU:HB2	2.02	0.59
1:C:126:LEU:HD12	1:C:149:GLU:HB3	1.84	0.59
1:B:313:ARG:HH21	1:B:334:PRO:HA	1.66	0.59
1:D:142:ILE:C	1:D:144:GLY:H	2.06	0.59
1:A:230:ALA:HA	1:A:296:SER:HB2	1.84	0.59
1:D:269:LYS:HG2	1:D:281:VAL:HG13	1.84	0.59
1:A:117:ASP:OD1	1:A:119:ARG:NH1	2.36	0.59
1:E:221:LEU:HD22	1:E:226:ALA:HA	1.84	0.59
1:G:115:HIS:C	1:A:117:ASP:OD2	2.42	0.58
1:F:283:VAL:HG22	1:F:284:ALA:H	1.68	0.58
1:B:183:GLU:HG3	1:B:313:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:HIS:NE2	1:F:123:THR:CG2	2.67	0.58
1:B:221:LEU:HD22	1:B:226:ALA:HA	1.86	0.58
1:D:239:ILE:HG13	1:D:240:ARG:H	1.68	0.58
1:F:126:LEU:HD12	1:F:149:GLU:HB3	1.85	0.58
1:F:191:ALA:HA	1:F:340:VAL:CG2	2.34	0.58
1:E:302:LYS:HE3	1:E:303:LEU:HB2	1.86	0.58
1:E:115:HIS:NE2	1:E:123:THR:HG22	2.19	0.58
1:D:283:VAL:HG13	1:D:284:ALA:N	2.18	0.58
1:C:192:ARG:NH2	1:C:286:ASP:OD2	2.36	0.58
1:B:242:VAL:O	1:B:245:PHE:HE1	1.86	0.58
1:B:313:ARG:HA	1:B:336:ALA:HA	1.85	0.58
1:A:245:PHE:CZ	1:A:300:THR:HG22	2.39	0.58
1:D:279:GLY:HA2	1:D:284:ALA:HA	1.85	0.58
1:E:279:GLY:HA2	1:E:284:ALA:HA	1.85	0.58
1:G:315:ASN:HD22	1:G:315:ASN:H	1.51	0.58
1:C:122:TYR:CB	1:C:308:LEU:HG	2.33	0.58
1:D:102:ALA:HB3	1:D:189:THR:HB	1.86	0.58
1:G:269:LYS:HG2	1:G:281:VAL:HG13	1.86	0.58
1:B:306:LEU:CB	1:B:343:LYS:HE3	2.34	0.57
1:D:194:ALA:CB	1:D:340:VAL:HG22	2.34	0.57
1:G:102:ALA:HB3	1:G:189:THR:HB	1.85	0.57
1:F:122:TYR:N	1:F:122:TYR:CD2	2.73	0.57
1:B:122:TYR:HB3	1:B:308:LEU:HG	1.85	0.57
1:E:306:LEU:CB	1:E:343:LYS:HE3	2.34	0.57
1:E:115:HIS:HB2	1:E:121:GLU:HB3	1.84	0.57
1:A:309:GLU:HA	1:A:338:GLY:HA3	1.86	0.57
1:F:231:LEU:O	1:F:235:GLU:HB2	2.04	0.57
1:A:279:GLY:HA2	1:A:284:ALA:HA	1.87	0.57
1:C:138:VAL:HG13	1:C:138:VAL:O	2.04	0.57
1:G:194:ALA:CB	1:G:340:VAL:HG22	2.35	0.57
1:D:194:ALA:HB3	1:D:340:VAL:HG21	1.87	0.57
1:G:115:HIS:HD2	1:G:121:GLU:HB3	1.69	0.57
1:E:163:THR:HG21	1:F:146:CYS:HA	1.86	0.57
1:E:115:HIS:NE2	1:E:123:THR:CG2	2.68	0.57
1:A:283:VAL:HG13	1:A:284:ALA:N	2.19	0.57
1:G:113:MET:HB2	1:G:123:THR:H	1.70	0.57
1:C:161:THR:HA	1:C:334:PRO:HD2	1.87	0.57
1:F:122:TYR:HD2	1:F:122:TYR:N	2.03	0.57
1:A:122:TYR:CD2	1:A:122:TYR:N	2.73	0.57
1:D:300:THR:C	1:D:302:LYS:HG3	2.24	0.57
1:C:308:LEU:HD12	1:C:308:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:VAL:HG22	1:G:284:ALA:H	1.70	0.57
1:C:115:HIS:NE2	1:C:123:THR:CG2	2.68	0.56
1:D:119:ARG:H	1:D:119:ARG:HD3	1.70	0.56
1:A:313:ARG:HH21	1:A:334:PRO:HA	1.70	0.56
1:D:110:GLU:CD	1:D:305:ASP:HB3	2.26	0.56
1:C:308:LEU:CD1	1:C:308:LEU:H	2.17	0.56
1:D:115:HIS:NE2	1:D:123:THR:HG22	2.20	0.56
1:F:279:GLY:HA2	1:F:284:ALA:HA	1.86	0.56
1:F:313:ARG:HD2	1:F:334:PRO:CB	2.25	0.56
1:D:161:THR:HA	1:D:334:PRO:HD2	1.87	0.56
1:E:300:THR:C	1:E:302:LYS:HG3	2.26	0.56
1:D:126:LEU:CD2	1:D:127:GLY:H	2.11	0.56
1:B:126:LEU:CA	1:B:302:LYS:HD2	2.30	0.56
1:A:125:GLN:HA	1:A:148:VAL:HG23	1.86	0.56
1:A:313:ARG:HD2	1:A:334:PRO:CB	2.28	0.56
1:E:194:ALA:HB3	1:E:340:VAL:HG21	1.87	0.56
1:D:122:TYR:HB3	1:D:308:LEU:HG	1.86	0.56
1:D:314:ALA:H	1:D:337:ALA:H	1.53	0.56
1:E:313:ARG:HH22	1:E:315:ASN:HB3	1.71	0.56
1:G:308:LEU:HD11	1:G:341:VAL:HG23	1.87	0.56
1:F:230:ALA:O	1:F:234:PRO:HD2	2.05	0.56
1:D:298:VAL:H	1:D:304:ARG:NH2	1.99	0.56
1:E:230:ALA:O	1:E:234:PRO:HD2	2.05	0.56
1:C:283:VAL:HG22	1:C:284:ALA:H	1.71	0.56
1:B:230:ALA:O	1:B:234:PRO:HD2	2.05	0.56
1:B:195:LEU:HD22	1:B:306:LEU:O	2.04	0.56
1:E:195:LEU:HD23	1:E:341:VAL:H	1.69	0.56
1:D:113:MET:HB2	1:D:123:THR:H	1.70	0.56
1:A:252:HIS:NE2	1:B:282:LYS:HA	2.20	0.56
1:A:235:GLU:O	1:A:238:SER:HB3	2.05	0.56
1:F:283:VAL:HG13	1:F:284:ALA:N	2.20	0.56
1:C:283:VAL:HG13	1:C:284:ALA:N	2.21	0.56
1:C:194:ALA:CB	1:C:340:VAL:CG2	2.84	0.56
1:G:314:ALA:H	1:G:337:ALA:H	1.54	0.56
1:A:283:VAL:HG22	1:A:284:ALA:H	1.70	0.56
1:F:221:LEU:HD22	1:F:226:ALA:HA	1.87	0.56
1:F:131:ALA:C	1:F:133:ALA:H	2.09	0.56
1:B:101:THR:HA	1:B:186:ALA:HA	1.87	0.56
1:A:194:ALA:HB3	1:A:340:VAL:HG21	1.85	0.56
1:E:195:LEU:HD22	1:E:306:LEU:O	2.05	0.56
1:B:315:ASN:ND2	1:B:315:ASN:H	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:LYS:HG3	1:F:303:LEU:H	1.71	0.56
1:C:106:ILE:H	1:C:192:ARG:HE	1.54	0.56
1:E:283:VAL:HG13	1:E:284:ALA:N	2.20	0.56
1:E:312:ARG:O	1:E:337:ALA:HB3	2.06	0.55
1:D:183:GLU:HG3	1:D:313:ARG:NH1	2.21	0.55
1:B:165:ILE:HA	1:B:329:HIS:HA	1.88	0.55
1:D:313:ARG:HH21	1:D:334:PRO:HA	1.71	0.55
1:G:183:GLU:HG3	1:G:313:ARG:NH1	2.20	0.55
1:E:283:VAL:HG22	1:E:284:ALA:H	1.72	0.55
1:F:309:GLU:HA	1:F:338:GLY:HA3	1.87	0.55
1:B:156:ILE:HB	1:C:135:ASP:HB2	1.86	0.55
1:D:313:ARG:HD2	1:D:334:PRO:CB	2.27	0.55
1:E:183:GLU:HG3	1:E:313:ARG:NH1	2.20	0.55
1:F:194:ALA:HA	1:F:342:PHE:CZ	2.41	0.55
1:C:298:VAL:O	1:C:300:THR:N	2.39	0.55
1:C:274:ALA:HA	1:C:287:ASN:HD22	1.70	0.55
1:A:128:GLU:HA	1:A:147:ASN:HB2	1.87	0.55
1:A:101:THR:HA	1:A:186:ALA:HA	1.88	0.55
1:F:313:ARG:HH21	1:F:334:PRO:HA	1.70	0.55
1:E:230:ALA:HA	1:E:296:SER:HB2	1.88	0.55
1:G:306:LEU:CB	1:G:343:LYS:HE3	2.37	0.55
1:B:194:ALA:HB3	1:B:340:VAL:HG21	1.87	0.55
1:B:197:LYS:HA	1:B:342:PHE:CE2	2.42	0.55
1:E:300:THR:HA	1:E:301:VAL:HG13	1.89	0.55
1:B:321:ILE:HB	1:B:324:LYS:HB2	1.88	0.55
1:G:301:VAL:N	1:G:302:LYS:HG2	2.22	0.55
1:B:302:LYS:HE3	1:B:303:LEU:H	1.72	0.55
1:C:221:LEU:HD22	1:C:226:ALA:HA	1.88	0.55
1:A:183:GLU:HG3	1:A:313:ARG:NH1	2.21	0.54
1:D:126:LEU:O	1:D:128:GLU:N	2.39	0.54
1:F:183:GLU:HG3	1:F:313:ARG:NH1	2.22	0.54
1:G:245:PHE:CZ	1:G:300:THR:CG2	2.88	0.54
1:B:198:ASN:H	1:B:342:PHE:HZ	1.54	0.54
1:G:283:VAL:HG13	1:G:284:ALA:N	2.22	0.54
1:B:283:VAL:HG13	1:B:284:ALA:N	2.23	0.54
1:C:113:MET:HB2	1:C:123:THR:H	1.73	0.54
1:D:230:ALA:O	1:D:234:PRO:HD2	2.08	0.54
1:B:213:SER:HA	1:B:304:ARG:NH2	2.21	0.54
1:F:242:VAL:O	1:F:245:PHE:HE1	1.90	0.54
1:E:300:THR:HA	1:E:301:VAL:CG1	2.38	0.54
1:D:197:LYS:HA	1:D:342:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLY:HA3	1:C:271:VAL:HG22	1.90	0.54
1:G:309:GLU:HA	1:G:338:GLY:HA3	1.89	0.54
1:D:129:SER:O	1:D:144:GLY:HA3	2.07	0.54
1:D:283:VAL:HG22	1:D:284:ALA:H	1.73	0.54
1:C:194:ALA:CB	1:C:340:VAL:HG22	2.38	0.54
1:A:314:ALA:H	1:A:337:ALA:H	1.54	0.54
1:C:125:GLN:HA	1:C:148:VAL:HG23	1.89	0.54
1:E:138:VAL:HG22	1:E:139:LEU:H	1.72	0.54
1:B:200:VAL:HG12	1:B:202:ALA:H	1.72	0.54
1:C:183:GLU:HG3	1:C:313:ARG:NH1	2.23	0.54
1:C:119:ARG:H	1:C:119:ARG:HD3	1.73	0.54
1:C:122:TYR:CD2	1:C:122:TYR:N	2.76	0.54
1:B:250:VAL:HG22	1:B:292:PHE:HB2	1.90	0.54
1:G:151:LYS:HG3	1:G:343:LYS:HG3	1.90	0.54
1:G:122:TYR:CD1	1:G:306:LEU:CG	2.80	0.53
1:C:180:LEU:HD23	1:C:312:ARG:HH22	1.73	0.53
1:F:294:HIS:CE1	1:F:295:ARG:HD2	2.44	0.53
1:E:315:ASN:ND2	1:E:315:ASN:H	2.05	0.53
1:B:122:TYR:HD2	1:B:122:TYR:N	2.07	0.53
1:D:221:LEU:HD23	1:D:295:ARG:HH11	1.73	0.53
1:G:150:SER:HB2	1:A:154:GLU:OE2	2.08	0.53
1:A:194:ALA:CB	1:A:340:VAL:HG22	2.38	0.53
1:F:247:VAL:HG23	1:F:280:ASN:HD22	1.73	0.53
1:D:125:GLN:O	1:D:302:LYS:HD2	2.07	0.53
1:C:159:LEU:HA	1:C:334:PRO:O	2.09	0.53
1:F:198:ASN:H	1:F:342:PHE:HZ	1.56	0.53
1:B:279:GLY:HA2	1:B:284:ALA:HA	1.90	0.53
1:F:247:VAL:H	1:F:280:ASN:ND2	2.07	0.53
1:D:122:TYR:N	1:D:122:TYR:CD2	2.77	0.53
1:B:126:LEU:HD23	1:B:302:LYS:HB2	1.91	0.53
1:F:113:MET:HG3	1:F:123:THR:OG1	2.08	0.53
1:C:275:ASN:H	1:C:287:ASN:HB2	1.74	0.53
1:F:166:GLU:HB2	1:F:328:GLY:HA3	1.91	0.53
1:E:165:ILE:HA	1:E:329:HIS:HA	1.90	0.53
1:F:161:THR:HA	1:F:334:PRO:HD2	1.90	0.53
1:G:126:LEU:HA	1:G:302:LYS:HB3	1.91	0.53
1:F:192:ARG:NH2	1:F:286:ASP:OD2	2.42	0.53
1:C:122:TYR:N	1:C:122:TYR:HD2	2.06	0.53
1:C:144:GLY:O	1:C:145:LEU:CB	2.56	0.53
1:C:126:LEU:HA	1:C:302:LYS:HD2	1.91	0.53
1:F:229:ALA:HB1	1:F:295:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:ASN:ND2	1:F:315:ASN:H	2.07	0.53
1:G:117:ASP:OD2	1:A:115:HIS:C	2.47	0.53
1:E:194:ALA:CB	1:E:340:VAL:HG22	2.38	0.53
1:C:213:SER:HA	1:C:304:ARG:NH2	2.23	0.53
1:A:195:LEU:HD23	1:A:341:VAL:N	2.15	0.53
1:F:110:GLU:CD	1:F:305:ASP:HB3	2.28	0.53
1:G:313:ARG:HD2	1:G:334:PRO:CB	2.29	0.53
1:A:229:ALA:HB1	1:A:295:ARG:HG3	1.90	0.53
1:G:239:ILE:O	1:G:241:ASN:N	2.41	0.53
1:G:119:ARG:H	1:A:119:ARG:HH22	1.56	0.52
1:F:308:LEU:HD21	1:F:339:ALA:HB3	1.90	0.52
1:E:193:ALA:HB1	1:E:198:ASN:HB2	1.91	0.52
1:C:156:ILE:HB	1:D:136:GLY:HA2	1.91	0.52
1:F:195:LEU:HD23	1:F:341:VAL:H	1.75	0.52
1:F:113:MET:HB2	1:F:123:THR:H	1.75	0.52
1:G:101:THR:HA	1:G:186:ALA:HA	1.92	0.52
1:B:125:GLN:HA	1:B:148:VAL:HG23	1.90	0.52
1:G:152:TYR:HB2	1:A:152:TYR:CE2	2.45	0.52
1:D:122:TYR:N	1:D:122:TYR:HD2	2.07	0.52
1:F:119:ARG:H	1:F:119:ARG:HD3	1.74	0.52
1:D:212:ASP:O	1:D:304:ARG:NH2	2.42	0.52
1:E:159:LEU:HD11	1:F:135:ASP:HB2	1.91	0.52
1:G:152:TYR:HB2	1:A:152:TYR:CD2	2.45	0.52
1:B:124:SER:HB3	1:B:306:LEU:HD13	1.91	0.52
1:E:122:TYR:CD2	1:E:122:TYR:N	2.78	0.52
1:B:301:VAL:N	1:B:302:LYS:HG3	2.25	0.52
1:A:221:LEU:HD23	1:A:295:ARG:HH11	1.75	0.52
1:E:101:THR:HA	1:E:186:ALA:HA	1.91	0.52
1:G:230:ALA:HA	1:G:296:SER:CB	2.40	0.52
1:D:301:VAL:N	1:D:302:LYS:CG	2.60	0.52
1:C:279:GLY:HA2	1:C:284:ALA:HA	1.92	0.52
1:A:110:GLU:CD	1:A:305:ASP:HB3	2.30	0.52
1:A:308:LEU:HD21	1:A:339:ALA:HB3	1.92	0.52
1:G:306:LEU:HB2	1:G:343:LYS:HE3	1.92	0.52
1:B:122:TYR:N	1:B:122:TYR:CD2	2.77	0.52
1:D:294:HIS:CE1	1:D:295:ARG:HD2	2.45	0.52
1:F:165:ILE:HA	1:F:329:HIS:HA	1.92	0.52
1:E:250:VAL:HG22	1:E:292:PHE:HB2	1.92	0.52
1:B:195:LEU:HG	1:B:340:VAL:HG23	1.93	0.52
1:D:230:ALA:HA	1:D:296:SER:CB	2.39	0.52
1:G:280:ASN:HB3	1:G:285:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:ALA:HB3	1:G:138:VAL:HB	1.92	0.52
1:A:294:HIS:CE1	1:A:295:ARG:HD2	2.44	0.52
1:D:101:THR:HA	1:D:186:ALA:HA	1.91	0.52
1:D:192:ARG:NH2	1:D:286:ASP:OD2	2.43	0.51
1:A:142:ILE:C	1:A:144:GLY:N	2.62	0.51
1:E:294:HIS:CE1	1:E:295:ARG:HD2	2.45	0.51
1:A:192:ARG:NH2	1:A:286:ASP:OD2	2.43	0.51
1:G:126:LEU:HD23	1:G:302:LYS:HB2	1.91	0.51
1:D:106:ILE:H	1:D:192:ARG:HE	1.57	0.51
1:A:122:TYR:HD2	1:A:122:TYR:N	2.07	0.51
1:C:165:ILE:HA	1:C:329:HIS:HA	1.93	0.51
1:E:200:VAL:HG12	1:E:202:ALA:H	1.76	0.51
1:A:234:PRO:HA	1:A:298:VAL:HG13	1.91	0.51
1:F:193:ALA:O	1:F:194:ALA:CB	2.57	0.51
1:E:198:ASN:H	1:E:342:PHE:HZ	1.59	0.51
1:E:197:LYS:HA	1:E:342:PHE:CE2	2.45	0.51
1:C:239:ILE:HG13	1:C:241:ASN:H	1.75	0.51
1:A:165:ILE:HA	1:A:329:HIS:HA	1.93	0.51
1:G:194:ALA:HB3	1:G:340:VAL:HG21	1.91	0.51
1:B:115:HIS:NE2	1:B:123:THR:CG2	2.73	0.51
1:B:230:ALA:HA	1:B:296:SER:HB2	1.92	0.51
1:B:157:GLU:HB3	1:B:336:ALA:C	2.31	0.51
1:B:314:ALA:H	1:B:337:ALA:H	1.58	0.51
1:D:107:TYR:HB2	1:D:192:ARG:HG2	1.93	0.51
1:G:119:ARG:NH2	1:A:119:ARG:HD2	2.26	0.51
1:F:103:ASP:O	1:F:192:ARG:CZ	2.59	0.51
1:B:197:LYS:HG3	1:B:215:SER:OG	2.11	0.51
1:E:195:LEU:HG	1:E:340:VAL:HG23	1.93	0.51
1:E:302:LYS:HE3	1:E:303:LEU:H	1.73	0.51
1:A:315:ASN:H	1:A:315:ASN:ND2	2.08	0.51
1:B:294:HIS:CE1	1:B:295:ARG:HD2	2.46	0.51
1:G:195:LEU:HD23	1:G:341:VAL:N	2.24	0.51
1:B:195:LEU:HD23	1:B:341:VAL:H	1.75	0.51
1:E:239:ILE:O	1:E:241:ASN:N	2.39	0.51
1:D:125:GLN:HA	1:D:148:VAL:HG23	1.93	0.51
1:G:285:LYS:HG2	1:G:286:ASP:N	2.26	0.51
1:D:229:ALA:HB1	1:D:295:ARG:HG3	1.92	0.51
1:C:102:ALA:HB3	1:C:189:THR:HB	1.93	0.51
1:E:273:PRO:HB3	1:F:282:LYS:CB	2.38	0.51
1:G:313:ARG:HH21	1:G:334:PRO:HA	1.75	0.51
1:A:184:ILE:HG23	1:A:185:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ILE:HA	1:D:329:HIS:HA	1.93	0.51
1:A:195:LEU:CD2	1:A:341:VAL:H	2.19	0.51
1:G:115:HIS:HB2	1:G:121:GLU:CB	2.40	0.51
1:G:117:ASP:CG	1:A:117:ASP:H	2.14	0.51
1:G:126:LEU:HA	1:G:302:LYS:HB2	1.92	0.51
1:C:301:VAL:H	1:C:302:LYS:CG	2.24	0.51
1:E:119:ARG:HD3	1:E:119:ARG:H	1.76	0.51
1:F:101:THR:HA	1:F:186:ALA:HA	1.93	0.51
1:G:106:ILE:HB	1:G:192:ARG:HB3	1.92	0.51
1:D:267:GLY:HA3	1:D:271:VAL:HG22	1.93	0.51
1:E:122:TYR:HD2	1:E:122:TYR:N	2.08	0.50
1:C:122:TYR:CD1	1:C:306:LEU:CG	2.88	0.50
1:C:194:ALA:C	1:C:342:PHE:CE2	2.84	0.50
1:E:192:ARG:NH2	1:E:286:ASP:OD2	2.44	0.50
1:B:161:THR:HA	1:B:333:ARG:HA	1.94	0.50
1:G:116:TYR:O	1:A:116:TYR:C	2.50	0.50
1:E:122:TYR:CB	1:E:308:LEU:HG	2.39	0.50
1:D:274:ALA:HA	1:D:287:ASN:HD22	1.76	0.50
1:D:126:LEU:HD22	1:D:127:GLY:N	2.13	0.50
1:D:128:GLU:HA	1:D:147:ASN:HB2	1.93	0.50
1:C:294:HIS:CE1	1:C:295:ARG:HD2	2.47	0.50
1:B:245:PHE:CZ	1:B:300:THR:HG22	2.47	0.50
1:D:285:LYS:HG2	1:D:286:ASP:N	2.26	0.50
1:B:289:ILE:HD13	1:C:239:ILE:HG22	1.94	0.50
1:D:249:GLU:O	1:D:287:ASN:HA	2.12	0.50
1:A:239:ILE:HG13	1:A:240:ARG:N	2.26	0.50
1:E:313:ARG:HA	1:E:336:ALA:HA	1.93	0.50
1:F:332:LEU:O	1:F:334:PRO:HD3	2.12	0.50
1:C:313:ARG:HD2	1:C:334:PRO:CB	2.27	0.50
1:D:315:ASN:H	1:D:315:ASN:ND2	2.10	0.50
1:F:200:VAL:HG12	1:F:202:ALA:H	1.77	0.50
1:G:122:TYR:CG	1:G:306:LEU:HG	2.46	0.49
1:F:298:VAL:O	1:F:300:THR:HG23	2.12	0.49
1:D:300:THR:O	1:D:302:LYS:HG3	2.12	0.49
1:A:285:LYS:HG2	1:A:286:ASP:N	2.27	0.49
1:A:238:SER:OG	1:F:275:ASN:OD1	2.30	0.49
1:E:308:LEU:O	1:E:309:GLU:HB3	2.12	0.49
1:A:184:ILE:HG13	1:A:312:ARG:HB2	1.94	0.49
1:D:239:ILE:CG1	1:D:240:ARG:H	2.22	0.49
1:B:317:GLN:HA	1:B:332:LEU:HA	1.95	0.49
1:G:147:ASN:HA	1:B:137:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ILE:HG23	1:E:185:ILE:H	1.77	0.49
1:D:110:GLU:OE2	1:D:306:LEU:N	2.45	0.49
1:G:249:GLU:O	1:G:287:ASN:HA	2.12	0.49
1:G:275:ASN:H	1:G:287:ASN:HB2	1.77	0.49
1:A:274:ALA:HA	1:A:287:ASN:HD22	1.78	0.49
1:D:309:GLU:HA	1:D:338:GLY:HA3	1.93	0.49
1:G:117:ASP:OD2	1:A:116:TYR:N	2.45	0.49
1:G:122:TYR:N	1:G:122:TYR:CD2	2.80	0.49
1:G:197:LYS:HA	1:G:342:PHE:CZ	2.47	0.49
1:C:229:ALA:HB1	1:C:295:ARG:HG3	1.95	0.49
1:D:275:ASN:H	1:D:287:ASN:HB2	1.76	0.49
1:G:194:ALA:C	1:G:342:PHE:CE2	2.85	0.49
1:F:314:ALA:H	1:F:337:ALA:H	1.59	0.49
1:G:106:ILE:H	1:G:192:ARG:HE	1.59	0.49
1:G:274:ALA:HA	1:G:287:ASN:HD22	1.78	0.49
1:B:298:VAL:O	1:B:300:THR:N	2.46	0.49
1:D:236:LYS:O	1:D:239:ILE:HG12	2.13	0.49
1:G:267:GLY:HA3	1:G:271:VAL:HG22	1.93	0.49
1:C:135:ASP:O	1:C:138:VAL:CG1	2.60	0.49
1:A:122:TYR:HB2	1:A:306:LEU:HG	1.93	0.49
1:F:194:ALA:HA	1:F:342:PHE:CE2	2.48	0.49
1:A:129:SER:O	1:A:144:GLY:HA3	2.12	0.49
1:A:129:SER:O	1:A:144:GLY:CA	2.60	0.49
1:C:110:GLU:CD	1:C:305:ASP:HB3	2.32	0.49
1:C:200:VAL:HG12	1:C:202:ALA:H	1.78	0.49
1:G:122:TYR:N	1:G:122:TYR:HD2	2.11	0.49
1:C:314:ALA:H	1:C:337:ALA:H	1.61	0.49
1:F:194:ALA:CB	1:F:340:VAL:CG2	2.91	0.49
1:F:147:ASN:O	1:F:148:VAL:HG12	2.13	0.49
1:C:313:ARG:HH21	1:C:334:PRO:HA	1.76	0.48
1:E:298:VAL:O	1:E:300:THR:HG23	2.13	0.48
1:D:280:ASN:HB3	1:D:285:LYS:HB2	1.93	0.48
1:A:157:GLU:HB2	1:A:335:GLU:HB3	1.94	0.48
1:B:184:ILE:HG23	1:B:185:ILE:H	1.78	0.48
1:G:294:HIS:CE1	1:G:295:ARG:HD2	2.47	0.48
1:C:101:THR:HA	1:C:186:ALA:HA	1.93	0.48
1:F:267:GLY:HA3	1:F:271:VAL:HG22	1.95	0.48
1:A:280:ASN:HB3	1:A:285:LYS:HB2	1.95	0.48
1:D:187:ALA:HB3	1:D:313:ARG:HB2	1.95	0.48
1:E:110:GLU:OE2	1:E:195:LEU:HB3	2.13	0.48
1:G:213:SER:HA	1:G:304:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH1	1:A:192:ARG:HB2	2.27	0.48
1:G:122:TYR:CB	1:G:308:LEU:HG	2.42	0.48
1:F:120:SER:HB2	1:F:308:LEU:HD23	1.93	0.48
1:B:115:HIS:HB2	1:B:121:GLU:HB3	1.95	0.48
1:D:184:ILE:HG23	1:D:185:ILE:H	1.79	0.48
1:A:110:GLU:OE2	1:A:306:LEU:N	2.47	0.48
1:F:221:LEU:HD23	1:F:295:ARG:HH11	1.77	0.48
1:C:258:ALA:HA	1:C:267:GLY:H	1.78	0.48
1:C:230:ALA:HA	1:C:296:SER:HB2	1.93	0.48
1:G:115:HIS:CE1	1:G:123:THR:CG2	2.96	0.48
1:F:234:PRO:HB2	1:F:282:LYS:HD2	1.95	0.48
1:C:195:LEU:HD22	1:C:306:LEU:O	2.13	0.48
1:B:273:PRO:HB3	1:C:282:LYS:CB	2.37	0.48
1:G:221:LEU:HD23	1:G:295:ARG:HH11	1.79	0.48
1:G:117:ASP:HB3	1:G:118:VAL:H	1.43	0.48
1:A:141:GLU:O	1:A:142:ILE:C	2.52	0.48
1:G:165:ILE:HA	1:G:329:HIS:HA	1.96	0.48
1:A:124:SER:HB3	1:A:306:LEU:HB2	1.94	0.48
1:D:126:LEU:HD12	1:D:149:GLU:HB3	1.95	0.48
1:D:194:ALA:C	1:D:342:PHE:CE2	2.87	0.48
1:C:115:HIS:NE2	1:C:123:THR:HG22	2.29	0.48
1:D:213:SER:HA	1:D:304:ARG:HH21	1.79	0.48
1:B:256:GLY:O	1:B:260:THR:HG22	2.14	0.48
1:A:267:GLY:HA3	1:A:271:VAL:HG22	1.96	0.48
1:G:117:ASP:HB2	1:A:119:ARG:NH2	2.29	0.48
1:A:189:THR:HA	1:A:192:ARG:HD3	1.95	0.48
1:G:119:ARG:HH21	1:G:121:GLU:CD	2.16	0.48
1:E:195:LEU:HD21	1:E:340:VAL:HA	1.96	0.48
1:F:285:LYS:HG2	1:F:286:ASP:N	2.29	0.48
1:A:126:LEU:HD22	1:A:127:GLY:H	1.79	0.48
1:C:221:LEU:HD23	1:C:295:ARG:HH11	1.77	0.48
1:A:249:GLU:O	1:A:287:ASN:HA	2.13	0.48
1:B:313:ARG:HH22	1:B:315:ASN:HB3	1.78	0.47
1:A:122:TYR:HD1	1:A:306:LEU:CG	2.17	0.47
1:C:157:GLU:O	1:C:159:LEU:HD12	2.14	0.47
1:C:184:ILE:HG23	1:C:185:ILE:H	1.78	0.47
1:F:280:ASN:HB3	1:F:285:LYS:HB2	1.96	0.47
1:E:110:GLU:OE2	1:E:306:LEU:N	2.46	0.47
1:D:194:ALA:HA	1:D:342:PHE:CZ	2.48	0.47
1:B:119:ARG:HD3	1:B:119:ARG:H	1.79	0.47
1:E:230:ALA:HA	1:E:296:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ALA:CA	1:C:138:VAL:HB	2.43	0.47
1:A:113:MET:HB2	1:A:123:THR:H	1.79	0.47
1:E:106:ILE:HB	1:E:192:ARG:HB3	1.96	0.47
1:E:106:ILE:H	1:E:192:ARG:HE	1.62	0.47
1:F:184:ILE:HG23	1:F:185:ILE:H	1.78	0.47
1:D:221:LEU:HD22	1:D:226:ALA:HA	1.96	0.47
1:B:168:THR:HG22	1:B:175:THR:HG21	1.97	0.47
1:E:156:ILE:HG12	1:F:136:GLY:HA2	1.96	0.47
1:F:213:SER:HA	1:F:304:ARG:NH2	2.28	0.47
1:F:106:ILE:HB	1:F:192:ARG:HB3	1.96	0.47
1:F:124:SER:HB3	1:F:306:LEU:HB2	1.97	0.47
1:D:235:GLU:O	1:D:238:SER:HB3	2.15	0.47
1:C:164:VAL:O	1:C:330:GLY:N	2.41	0.47
1:D:252:HIS:HE2	1:E:282:LYS:HA	1.80	0.47
1:G:153:ASN:ND2	1:G:341:VAL:CG2	2.65	0.47
1:A:221:LEU:HD22	1:A:226:ALA:HA	1.96	0.47
1:C:257:GLY:HA2	1:C:262:ARG:CG	2.45	0.47
1:A:191:ALA:HA	1:A:340:VAL:CB	2.44	0.47
1:A:228:TYR:C	1:A:230:ALA:N	2.68	0.47
1:B:194:ALA:HA	1:B:342:PHE:CE2	2.50	0.47
1:C:147:ASN:O	1:C:148:VAL:HG12	2.15	0.47
1:A:192:ARG:HB2	1:A:192:ARG:CZ	2.43	0.47
1:A:338:GLY:O	1:A:339:ALA:HB2	2.15	0.47
1:F:126:LEU:HD23	1:F:302:LYS:HB2	1.97	0.47
1:D:122:TYR:CD1	1:D:306:LEU:CG	2.90	0.47
1:C:193:ALA:O	1:C:194:ALA:HB2	2.15	0.47
1:D:227:ASN:HB3	1:D:228:TYR:H	1.41	0.47
1:C:242:VAL:O	1:C:245:PHE:CE1	2.68	0.47
1:E:107:TYR:HB2	1:E:192:ARG:HG2	1.97	0.47
1:A:184:ILE:HG23	1:A:185:ILE:N	2.30	0.47
1:E:221:LEU:HD23	1:E:295:ARG:HH11	1.80	0.47
1:B:221:LEU:HD23	1:B:295:ARG:HH11	1.79	0.47
1:C:221:LEU:HD23	1:C:295:ARG:NH1	2.29	0.47
1:E:125:GLN:HA	1:E:148:VAL:HG23	1.96	0.47
1:G:250:VAL:HG23	1:G:253:LEU:H	1.80	0.47
1:F:159:LEU:HA	1:F:334:PRO:O	2.15	0.47
1:E:191:ALA:O	1:E:195:LEU:N	2.47	0.47
1:E:228:TYR:C	1:E:230:ALA:N	2.68	0.47
1:A:212:ASP:O	1:A:304:ARG:NH2	2.48	0.47
1:E:166:GLU:HB2	1:E:328:GLY:HA3	1.96	0.47
1:E:197:LYS:HG3	1:E:215:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASN:HB3	1:E:285:LYS:HB2	1.97	0.47
1:F:102:ALA:HB3	1:F:189:THR:HB	1.97	0.47
1:E:180:LEU:HD23	1:E:312:ARG:HH22	1.80	0.46
1:F:313:ARG:HH22	1:F:315:ASN:HB3	1.80	0.46
1:D:195:LEU:HD22	1:D:306:LEU:O	2.16	0.46
1:F:119:ARG:HE	1:F:121:GLU:CG	2.28	0.46
1:C:285:LYS:HG2	1:C:286:ASP:N	2.30	0.46
1:F:227:ASN:HB3	1:F:228:TYR:H	1.43	0.46
1:B:106:ILE:HB	1:B:192:ARG:HB3	1.96	0.46
1:G:212:ASP:O	1:G:304:ARG:NH2	2.48	0.46
1:F:104:VAL:HG23	1:F:185:ILE:HG23	1.97	0.46
1:D:250:VAL:HG23	1:D:253:LEU:H	1.80	0.46
1:A:230:ALA:HA	1:A:296:SER:CB	2.43	0.46
1:B:122:TYR:CD1	1:B:306:LEU:CG	2.89	0.46
1:B:122:TYR:CB	1:B:308:LEU:HG	2.45	0.46
1:E:137:ALA:HA	1:E:138:VAL:HA	1.73	0.46
1:E:184:ILE:HG13	1:E:312:ARG:HB2	1.96	0.46
1:C:161:THR:HG21	1:D:142:ILE:HD13	1.98	0.46
1:F:275:ASN:H	1:F:287:ASN:HB2	1.79	0.46
1:B:192:ARG:NH2	1:B:286:ASP:OD2	2.48	0.46
1:C:194:ALA:CA	1:C:342:PHE:CE2	2.99	0.46
1:G:184:ILE:HG23	1:G:185:ILE:N	2.30	0.46
1:B:248:VAL:CG2	1:B:288:VAL:HG22	2.45	0.46
1:E:229:ALA:HB1	1:E:295:ARG:HG3	1.97	0.46
1:G:221:LEU:HD22	1:G:226:ALA:HA	1.96	0.46
1:F:112:ALA:HA	1:F:307:ALA:O	2.15	0.46
1:E:267:GLY:HA3	1:E:271:VAL:HG22	1.96	0.46
1:G:184:ILE:HG23	1:G:185:ILE:H	1.79	0.46
1:F:180:LEU:HD23	1:F:312:ARG:HH22	1.81	0.46
1:F:161:THR:HA	1:F:333:ARG:HA	1.97	0.46
1:B:110:GLU:OE2	1:B:195:LEU:HB3	2.16	0.46
1:D:122:TYR:CB	1:D:308:LEU:HG	2.45	0.46
1:C:121:GLU:O	1:C:308:LEU:HB3	2.16	0.46
1:C:242:VAL:O	1:C:245:PHE:HE1	1.98	0.46
1:B:289:ILE:HB	1:C:239:ILE:HA	1.97	0.46
1:G:229:ALA:HB1	1:G:295:ARG:HG3	1.97	0.46
1:A:113:MET:HG3	1:A:123:THR:OG1	2.16	0.46
1:B:193:ALA:HB1	1:B:198:ASN:HB2	1.97	0.46
1:G:187:ALA:HB3	1:G:313:ARG:HB2	1.97	0.46
1:F:184:ILE:HG23	1:F:185:ILE:N	2.31	0.46
1:A:122:TYR:CD1	1:A:306:LEU:CG	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:LYS:HD2	1:G:345:GLU:HB3	1.98	0.45
1:C:184:ILE:HD12	1:C:312:ARG:HD3	1.98	0.45
1:F:194:ALA:CA	1:F:342:PHE:CE2	3.00	0.45
1:B:153:ASN:CG	1:B:341:VAL:HG21	2.36	0.45
1:B:301:VAL:H	1:B:302:LYS:CG	2.25	0.45
1:C:191:ALA:O	1:C:195:LEU:HG	2.16	0.45
1:C:343:LYS:HB2	1:C:343:LYS:HZ3	1.82	0.45
1:F:184:ILE:HG13	1:F:312:ARG:HB2	1.98	0.45
1:E:159:LEU:HA	1:E:335:GLU:HA	1.97	0.45
1:E:314:ALA:H	1:E:337:ALA:H	1.64	0.45
1:B:191:ALA:O	1:B:195:LEU:N	2.49	0.45
1:D:308:LEU:HD13	1:D:340:VAL:N	2.30	0.45
1:C:193:ALA:O	1:C:194:ALA:CB	2.65	0.45
1:B:117:ASP:HB2	1:B:119:ARG:HD3	1.98	0.45
1:D:184:ILE:HG23	1:D:185:ILE:N	2.31	0.45
1:C:128:GLU:HB2	1:C:130:LEU:CD2	2.40	0.45
1:G:115:HIS:CB	1:A:117:ASP:OD2	2.64	0.45
1:G:122:TYR:HB2	1:G:306:LEU:HG	1.98	0.45
1:F:195:LEU:HG	1:F:340:VAL:HG23	1.98	0.45
1:B:285:LYS:HG2	1:B:286:ASP:N	2.31	0.45
1:D:193:ALA:HB1	1:D:198:ASN:HB2	1.99	0.45
1:D:228:TYR:C	1:D:230:ALA:N	2.69	0.45
1:A:275:ASN:H	1:A:287:ASN:HB2	1.81	0.45
1:A:200:VAL:HG12	1:A:202:ALA:H	1.81	0.45
1:E:335:GLU:O	1:E:337:ALA:N	2.50	0.45
1:A:195:LEU:HD22	1:A:306:LEU:O	2.17	0.45
1:C:315:ASN:ND2	1:C:315:ASN:H	2.13	0.45
1:B:308:LEU:HD13	1:B:340:VAL:N	2.32	0.45
1:D:119:ARG:HE	1:D:121:GLU:HG3	1.80	0.45
1:D:239:ILE:CG1	1:D:240:ARG:N	2.76	0.45
1:F:312:ARG:O	1:F:337:ALA:HB3	2.16	0.45
1:A:250:VAL:HB	1:A:252:HIS:HD1	1.80	0.45
1:B:166:GLU:HB2	1:B:328:GLY:HA3	1.98	0.45
1:G:119:ARG:HD2	1:G:152:TYR:CE2	2.51	0.45
1:D:283:VAL:HG13	1:D:284:ALA:H	1.81	0.45
1:B:267:GLY:HA3	1:B:271:VAL:HG22	1.98	0.45
1:A:110:GLU:OE2	1:A:195:LEU:HB3	2.16	0.45
1:G:103:ASP:O	1:G:192:ARG:CZ	2.64	0.45
1:B:115:HIS:CD2	1:B:121:GLU:HB3	2.52	0.45
1:E:161:THR:HB	1:E:333:ARG:HE	1.82	0.45
1:G:308:LEU:HD13	1:G:340:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:TYR:CD1	1:F:306:LEU:CG	2.89	0.45
1:G:161:THR:HA	1:G:334:PRO:HD2	1.99	0.45
1:G:105:LEU:H	1:G:192:ARG:HE	1.64	0.45
1:E:187:ALA:HB3	1:E:313:ARG:HB2	1.98	0.45
1:C:194:ALA:HB1	1:C:340:VAL:HG22	1.99	0.45
1:F:221:LEU:HD23	1:F:295:ARG:NH1	2.31	0.45
1:B:161:THR:HA	1:B:334:PRO:HD2	1.98	0.45
1:B:184:ILE:HG23	1:B:185:ILE:N	2.31	0.45
1:E:301:VAL:HG22	1:E:302:LYS:HG2	1.99	0.45
1:E:117:ASP:HB2	1:E:119:ARG:HD3	1.99	0.45
1:C:103:ASP:O	1:C:192:ARG:CZ	2.65	0.44
1:C:269:LYS:HD3	1:C:280:ASN:HA	1.98	0.44
1:C:315:ASN:H	1:C:315:ASN:HD22	1.65	0.44
1:F:195:LEU:HD22	1:F:306:LEU:O	2.17	0.44
1:E:241:ASN:HD21	1:E:300:THR:HG21	1.81	0.44
1:C:245:PHE:CZ	1:C:300:THR:CG2	3.00	0.44
1:F:256:GLY:O	1:F:260:THR:HG22	2.18	0.44
1:E:285:LYS:HG2	1:E:286:ASP:N	2.32	0.44
1:G:115:HIS:CE1	1:G:123:THR:HG23	2.51	0.44
1:F:194:ALA:C	1:F:342:PHE:CE2	2.90	0.44
1:D:157:GLU:HB2	1:D:335:GLU:HB3	1.99	0.44
1:E:317:GLN:HA	1:E:332:LEU:HA	1.99	0.44
1:G:157:GLU:HB2	1:G:335:GLU:HB3	1.99	0.44
1:B:195:LEU:HD21	1:B:340:VAL:HA	1.98	0.44
1:C:113:MET:HG3	1:C:123:THR:OG1	2.18	0.44
1:C:301:VAL:HG12	1:C:302:LYS:HG2	1.99	0.44
1:C:249:GLU:O	1:C:287:ASN:HA	2.17	0.44
1:A:115:HIS:NE2	1:A:123:THR:CG2	2.81	0.44
1:A:119:ARG:CG	1:A:120:SER:N	2.73	0.44
1:E:122:TYR:CD1	1:E:306:LEU:CG	2.90	0.44
1:E:308:LEU:HD13	1:E:340:VAL:N	2.32	0.44
1:E:126:LEU:HB2	1:E:147:ASN:O	2.17	0.44
1:C:245:PHE:CZ	1:C:300:THR:HG22	2.53	0.44
1:E:268:GLN:HB3	1:E:269:LYS:H	1.63	0.44
1:G:107:TYR:HB2	1:G:192:ARG:HG2	2.00	0.44
1:G:117:ASP:OD2	1:A:121:GLU:HB2	2.18	0.44
1:A:119:ARG:NE	1:A:121:GLU:HG3	2.31	0.44
1:G:125:GLN:O	1:G:127:GLY:N	2.47	0.44
1:C:184:ILE:HG23	1:C:185:ILE:N	2.32	0.44
1:C:302:LYS:HG3	1:C:303:LEU:H	1.82	0.44
1:G:308:LEU:N	1:G:308:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:GLN:HB3	1:F:269:LYS:H	1.64	0.44
1:G:315:ASN:H	1:G:315:ASN:ND2	2.15	0.44
1:E:256:GLY:O	1:E:260:THR:HG22	2.18	0.44
1:B:321:ILE:HB	1:B:324:LYS:HD3	2.00	0.44
1:D:221:LEU:HD23	1:D:295:ARG:NH1	2.32	0.44
1:G:110:GLU:OE2	1:G:306:LEU:N	2.50	0.44
1:D:308:LEU:HD13	1:D:339:ALA:C	2.38	0.44
1:D:343:LYS:HD3	1:D:343:LYS:N	2.33	0.44
1:B:302:LYS:HG3	1:B:302:LYS:H	1.50	0.44
1:C:258:ALA:HA	1:C:267:GLY:N	2.32	0.44
1:B:187:ALA:HB3	1:B:313:ARG:HB2	2.00	0.44
1:B:107:TYR:HB2	1:B:192:ARG:HG2	2.00	0.44
1:G:268:GLN:HB3	1:G:269:LYS:H	1.63	0.44
1:C:230:ALA:HA	1:C:296:SER:CB	2.48	0.44
1:D:310:ARG:NH2	1:D:311:ALA:HB2	2.33	0.44
1:F:232:ILE:O	1:F:232:ILE:HG13	2.16	0.44
1:G:300:THR:O	1:G:302:LYS:HG2	2.18	0.43
1:F:230:ALA:HA	1:F:296:SER:CB	2.48	0.43
1:C:131:ALA:HB2	1:C:144:GLY:N	2.33	0.43
1:E:251:PRO:CB	1:F:235:GLU:HG2	2.48	0.43
1:G:310:ARG:NH2	1:G:311:ALA:HB2	2.33	0.43
1:E:184:ILE:HG23	1:E:185:ILE:N	2.33	0.43
1:B:161:THR:O	1:C:130:LEU:HD22	2.18	0.43
1:A:198:ASN:H	1:A:342:PHE:HZ	1.65	0.43
1:A:245:PHE:CZ	1:A:300:THR:CG2	3.01	0.43
1:G:213:SER:HA	1:G:304:ARG:HH21	1.81	0.43
1:C:232:ILE:O	1:C:232:ILE:HG13	2.18	0.43
1:A:119:ARG:NH2	1:A:121:GLU:HG3	2.32	0.43
1:C:335:GLU:O	1:C:337:ALA:N	2.51	0.43
1:F:249:GLU:O	1:F:287:ASN:HA	2.17	0.43
1:C:122:TYR:HB3	1:C:308:LEU:CB	2.48	0.43
1:G:221:LEU:HD23	1:G:295:ARG:NH1	2.33	0.43
1:D:237:GLY:HA2	1:D:241:ASN:HD22	1.83	0.43
1:B:184:ILE:HG13	1:B:312:ARG:HB2	1.98	0.43
1:G:301:VAL:O	1:G:305:ASP:HB2	2.16	0.43
1:F:247:VAL:HG22	1:F:296:SER:HB3	2.00	0.43
1:B:192:ARG:HB2	1:B:192:ARG:NH1	2.34	0.43
1:B:221:LEU:HD23	1:B:295:ARG:NH1	2.33	0.43
1:B:230:ALA:HA	1:B:296:SER:CB	2.48	0.43
1:E:333:ARG:HG2	1:E:335:GLU:HG3	1.99	0.43
1:A:117:ASP:HB3	1:A:118:VAL:H	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ARG:O	1:C:337:ALA:HB3	2.17	0.43
1:B:153:ASN:ND2	1:B:341:VAL:HG21	2.34	0.43
1:B:308:LEU:HD13	1:B:339:ALA:C	2.39	0.43
1:B:113:MET:HB2	1:B:123:THR:H	1.83	0.43
1:G:117:ASP:CB	1:A:119:ARG:NH2	2.82	0.43
1:B:110:GLU:CD	1:B:305:ASP:HB3	2.38	0.43
1:C:306:LEU:HB2	1:C:343:LYS:HE3	2.00	0.43
1:D:117:ASP:HB2	1:D:119:ARG:HD3	2.01	0.43
1:D:243:MET:SD	1:D:282:LYS:HD3	2.58	0.43
1:B:269:LYS:HD3	1:B:280:ASN:HA	2.01	0.43
1:F:115:HIS:NE2	1:F:123:THR:HG22	2.33	0.43
1:C:195:LEU:HD21	1:C:340:VAL:HA	2.01	0.43
1:C:195:LEU:HD23	1:C:341:VAL:H	1.84	0.43
1:D:244:GLY:HA2	1:D:282:LYS:HG3	2.00	0.43
1:B:255:ALA:HB2	1:C:235:GLU:OE2	2.18	0.43
1:C:125:GLN:O	1:C:302:LYS:HD2	2.18	0.43
1:G:116:TYR:N	1:A:117:ASP:OD2	2.52	0.43
1:G:119:ARG:HG3	1:G:153:ASN:O	2.19	0.43
1:C:184:ILE:HG13	1:C:312:ARG:HB2	2.01	0.43
1:E:258:ALA:HA	1:E:267:GLY:H	1.84	0.43
1:D:131:ALA:C	1:D:133:ALA:H	2.22	0.43
1:B:159:LEU:HB2	1:C:132:MET:O	2.19	0.43
1:B:180:LEU:HD23	1:B:312:ARG:HH22	1.83	0.43
1:C:313:ARG:HA	1:C:337:ALA:H	1.82	0.43
1:E:343:LYS:HB2	1:E:343:LYS:HZ3	1.84	0.43
1:D:188:LEU:O	1:D:192:ARG:HG3	2.19	0.43
1:G:227:ASN:HB3	1:G:228:TYR:H	1.37	0.43
1:G:308:LEU:HD13	1:G:339:ALA:C	2.39	0.43
1:F:198:ASN:HB3	1:F:199:TYR:H	1.69	0.43
1:F:242:VAL:O	1:F:245:PHE:CE1	2.72	0.43
1:C:194:ALA:HA	1:C:342:PHE:CE2	2.53	0.43
1:A:126:LEU:CA	1:A:302:LYS:HB2	2.37	0.43
1:E:289:ILE:HB	1:F:239:ILE:HA	2.01	0.43
1:A:137:ALA:HA	1:A:138:VAL:HA	1.78	0.43
1:A:211:PRO:HB3	1:A:214:TYR:HA	2.00	0.43
1:G:119:ARG:HD3	1:A:119:ARG:NH2	2.34	0.42
1:G:194:ALA:HA	1:G:342:PHE:CZ	2.54	0.42
1:C:313:ARG:HH22	1:C:315:ASN:HB3	1.84	0.42
1:F:151:LYS:HG3	1:F:343:LYS:HG3	2.01	0.42
1:E:298:VAL:O	1:E:300:THR:N	2.52	0.42
1:B:242:VAL:O	1:B:245:PHE:CE1	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ALA:HB2	1:C:144:GLY:H	1.83	0.42
1:F:137:ALA:HA	1:F:138:VAL:HA	1.76	0.42
1:B:163:THR:OG1	1:B:329:HIS:CE1	2.72	0.42
1:D:200:VAL:HG12	1:D:202:ALA:H	1.83	0.42
1:G:195:LEU:HD22	1:G:306:LEU:O	2.19	0.42
1:E:198:ASN:HB3	1:E:199:TYR:H	1.66	0.42
1:E:110:GLU:CD	1:E:305:ASP:HB3	2.39	0.42
1:E:308:LEU:HD13	1:E:339:ALA:C	2.40	0.42
1:F:117:ASP:HB2	1:F:119:ARG:HD3	2.01	0.42
1:G:228:TYR:C	1:G:230:ALA:N	2.72	0.42
1:B:227:ASN:HB3	1:B:228:TYR:H	1.37	0.42
1:B:157:GLU:HG2	1:B:337:ALA:HA	2.01	0.42
1:G:125:GLN:O	1:G:302:LYS:HB3	2.19	0.42
1:B:198:ASN:HB3	1:B:199:TYR:H	1.63	0.42
1:C:110:GLU:OE2	1:C:306:LEU:N	2.52	0.42
1:C:280:ASN:HB3	1:C:285:LYS:HB2	2.01	0.42
1:D:103:ASP:O	1:D:192:ARG:CZ	2.67	0.42
1:A:104:VAL:HG23	1:A:185:ILE:HG23	2.01	0.42
1:B:229:ALA:HB1	1:B:295:ARG:HG3	2.01	0.42
1:F:258:ALA:HA	1:F:267:GLY:H	1.84	0.42
1:G:191:ALA:O	1:G:195:LEU:N	2.53	0.42
1:D:113:MET:HG3	1:D:123:THR:OG1	2.19	0.42
1:A:120:SER:HB2	1:A:308:LEU:HD21	1.98	0.42
1:A:193:ALA:HB1	1:A:198:ASN:HB2	2.00	0.42
1:B:275:ASN:OD1	1:B:287:ASN:O	2.37	0.42
1:B:240:ARG:HD3	1:B:241:ASN:N	2.35	0.42
1:E:113:MET:HG3	1:E:123:THR:OG1	2.19	0.42
1:B:243:MET:HB2	1:B:282:LYS:HD2	2.01	0.42
1:F:258:ALA:HA	1:F:267:GLY:N	2.35	0.42
1:D:166:GLU:HB2	1:D:328:GLY:HA3	2.01	0.42
1:C:142:ILE:O	1:C:142:ILE:HG13	2.19	0.42
1:G:341:VAL:HG12	1:G:342:PHE:N	2.35	0.42
1:B:106:ILE:H	1:B:192:ARG:HE	1.67	0.42
1:B:280:ASN:HB3	1:B:285:LYS:HB2	2.00	0.42
1:E:195:LEU:HD23	1:E:341:VAL:N	2.32	0.42
1:E:194:ALA:C	1:E:342:PHE:CE2	2.93	0.42
1:C:192:ARG:O	1:C:196:THR:OG1	2.36	0.42
1:E:188:LEU:O	1:E:192:ARG:HG3	2.20	0.42
1:F:184:ILE:HD12	1:F:312:ARG:HD3	2.00	0.42
1:B:184:ILE:HB	1:B:312:ARG:HH11	1.84	0.42
1:G:152:TYR:CD2	1:G:153:ASN:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:HB3	1:A:313:ARG:HB2	2.01	0.42
1:F:269:LYS:HD3	1:F:280:ASN:HA	2.00	0.42
1:B:194:ALA:C	1:B:342:PHE:CE2	2.92	0.42
1:E:153:ASN:CG	1:E:341:VAL:HG21	2.40	0.42
1:G:313:ARG:HH22	1:G:315:ASN:HB3	1.83	0.42
1:E:269:LYS:HD3	1:E:280:ASN:HA	2.02	0.42
1:F:335:GLU:O	1:F:337:ALA:N	2.53	0.42
1:G:194:ALA:HA	1:G:342:PHE:CE2	2.54	0.42
1:F:106:ILE:O	1:F:110:GLU:HB3	2.19	0.42
1:F:301:VAL:H	1:F:302:LYS:HG2	1.83	0.42
1:E:127:GLY:O	1:E:147:ASN:HB2	2.19	0.42
1:D:149:GLU:OE2	1:D:343:LYS:HE2	2.20	0.42
1:A:142:ILE:O	1:A:144:GLY:N	2.53	0.42
1:E:226:ALA:CB	1:E:293:MET:SD	3.08	0.42
1:B:228:TYR:C	1:B:230:ALA:N	2.73	0.42
1:E:211:PRO:HB3	1:E:214:TYR:HA	2.02	0.42
1:C:166:GLU:HB2	1:C:328:GLY:HA3	2.02	0.42
1:A:310:ARG:NH2	1:A:311:ALA:HB2	2.35	0.42
1:B:211:PRO:HB3	1:B:214:TYR:HA	2.02	0.42
1:A:269:LYS:HD3	1:A:280:ASN:HA	2.01	0.42
1:G:115:HIS:HB2	1:G:121:GLU:HB2	2.00	0.42
1:F:106:ILE:H	1:F:192:ARG:HE	1.66	0.42
1:A:126:LEU:HG	1:A:149:GLU:CD	2.39	0.42
1:G:270:HIS:CE1	1:G:280:ASN:O	2.72	0.42
1:D:184:ILE:HG13	1:D:312:ARG:HB2	2.02	0.42
1:E:258:ALA:HA	1:E:267:GLY:N	2.35	0.42
1:C:233:ASP:CB	1:C:234:PRO:HD3	2.50	0.42
1:C:256:GLY:O	1:C:260:THR:HG22	2.19	0.42
1:C:126:LEU:HA	1:C:302:LYS:HB2	2.01	0.42
1:F:126:LEU:HB3	1:F:127:GLY:H	1.45	0.41
1:F:149:GLU:OE2	1:F:343:LYS:HE2	2.19	0.41
1:G:280:ASN:HB3	1:G:285:LYS:CB	2.50	0.41
1:E:227:ASN:HB3	1:E:228:TYR:H	1.43	0.41
1:F:248:VAL:CG2	1:F:288:VAL:HG22	2.50	0.41
1:D:211:PRO:HB3	1:D:214:TYR:HA	2.02	0.41
1:E:103:ASP:O	1:E:192:ARG:CZ	2.69	0.41
1:C:257:GLY:HA2	1:C:262:ARG:HG3	2.00	0.41
1:A:243:MET:SD	1:A:282:LYS:HD3	2.60	0.41
1:F:211:PRO:HB3	1:F:214:TYR:HA	2.02	0.41
1:A:194:ALA:HA	1:A:342:PHE:CE2	2.55	0.41
1:F:247:VAL:HG23	1:F:280:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:OD1	1:B:275:ASN:HA	2.19	0.41
1:E:113:MET:HB2	1:E:123:THR:H	1.84	0.41
1:F:144:GLY:O	1:F:145:LEU:CB	2.59	0.41
1:D:106:ILE:HB	1:D:192:ARG:HB3	2.02	0.41
1:B:136:GLY:C	1:B:137:ALA:O	2.58	0.41
1:E:313:ARG:HA	1:E:337:ALA:H	1.85	0.41
1:B:103:ASP:O	1:B:192:ARG:CZ	2.68	0.41
1:B:106:ILE:O	1:B:110:GLU:HB3	2.20	0.41
1:C:248:VAL:CG2	1:C:288:VAL:HG22	2.50	0.41
1:C:141:GLU:O	1:C:143:ALA:N	2.53	0.41
1:F:317:GLN:HE22	1:F:317:GLN:HB2	1.28	0.41
1:G:306:LEU:HB3	1:G:343:LYS:HE3	2.02	0.41
1:C:161:THR:HA	1:C:333:ARG:HA	2.02	0.41
1:F:195:LEU:HD21	1:F:340:VAL:HA	2.02	0.41
1:E:241:ASN:OD1	1:E:300:THR:HG21	2.20	0.41
1:B:119:ARG:HE	1:B:121:GLU:HG3	1.84	0.41
1:E:221:LEU:HD23	1:E:295:ARG:NH1	2.35	0.41
1:B:335:GLU:O	1:B:337:ALA:N	2.54	0.41
1:B:188:LEU:O	1:B:192:ARG:HG3	2.21	0.41
1:B:308:LEU:O	1:B:309:GLU:HB3	2.20	0.41
1:F:100:LEU:HA	1:F:190:LYS:HE2	2.01	0.41
1:G:138:VAL:O	1:G:138:VAL:HG13	2.20	0.41
1:F:126:LEU:CA	1:F:302:LYS:HD2	2.47	0.41
1:B:193:ALA:HB1	1:B:198:ASN:CB	2.51	0.41
1:E:124:SER:HB3	1:E:306:LEU:HD13	2.03	0.41
1:A:166:GLU:HB2	1:A:328:GLY:HA3	2.01	0.41
1:A:115:HIS:HD2	1:A:121:GLU:HB3	1.84	0.41
1:G:191:ALA:HA	1:G:340:VAL:CB	2.50	0.41
1:D:142:ILE:C	1:D:144:GLY:N	2.73	0.41
1:C:124:SER:HB3	1:C:306:LEU:HD13	2.03	0.41
1:G:234:PRO:HB2	1:G:282:LYS:HD2	2.02	0.41
1:C:317:GLN:HA	1:C:332:LEU:HA	2.02	0.41
1:A:343:LYS:N	1:A:343:LYS:HD3	2.36	0.41
1:C:104:VAL:HG23	1:C:185:ILE:HG23	2.02	0.41
1:A:302:LYS:CG	1:A:303:LEU:N	2.83	0.41
1:D:234:PRO:HB2	1:D:282:LYS:HD2	2.03	0.41
1:D:269:LYS:HD3	1:D:280:ASN:HA	2.03	0.41
1:D:280:ASN:HB3	1:D:285:LYS:CB	2.51	0.41
1:A:312:ARG:O	1:A:337:ALA:HB3	2.21	0.41
1:G:137:ALA:HB1	1:G:138:VAL:CB	2.48	0.41
1:A:250:VAL:HG23	1:A:253:LEU:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:TYR:C	1:C:230:ALA:N	2.75	0.41
1:C:128:GLU:O	1:C:130:LEU:HG	2.21	0.41
1:C:313:ARG:HA	1:C:337:ALA:N	2.36	0.41
1:E:239:ILE:HG13	1:E:239:ILE:H	1.75	0.41
1:E:192:ARG:NH1	1:E:192:ARG:HB2	2.36	0.41
1:C:162:ALA:HA	1:D:130:LEU:HD22	2.03	0.41
1:A:298:VAL:O	1:A:300:THR:N	2.54	0.40
1:A:304:ARG:O	1:A:342:PHE:HA	2.21	0.40
1:D:149:GLU:OE1	1:D:343:LYS:HG2	2.20	0.40
1:B:245:PHE:CZ	1:B:300:THR:CG2	3.04	0.40
1:E:313:ARG:CD	1:E:334:PRO:HB3	2.22	0.40
1:B:104:VAL:HG23	1:B:185:ILE:HG23	2.03	0.40
1:A:191:ALA:HA	1:A:340:VAL:HB	2.03	0.40
1:A:193:ALA:HB1	1:A:198:ASN:CB	2.50	0.40
1:G:100:LEU:HA	1:G:190:LYS:HE2	2.04	0.40
1:E:239:ILE:C	1:E:241:ASN:N	2.74	0.40
1:D:308:LEU:N	1:D:308:LEU:HD12	2.36	0.40
1:D:197:LYS:HD2	1:D:345:GLU:HB3	2.02	0.40
1:C:122:TYR:HB2	1:C:306:LEU:HG	2.02	0.40
1:A:221:LEU:HD23	1:A:295:ARG:NH1	2.34	0.40
1:G:226:ALA:HB3	1:G:293:MET:SD	2.62	0.40
1:G:184:ILE:HG13	1:G:312:ARG:HB2	2.04	0.40
1:B:313:ARG:HA	1:B:337:ALA:N	2.36	0.40
1:F:103:ASP:OD1	1:F:275:ASN:HA	2.21	0.40
1:B:248:VAL:HA	1:B:286:ASP:O	2.21	0.40
1:B:343:LYS:HB2	1:B:343:LYS:HZ3	1.86	0.40
1:E:171:LYS:HE2	1:F:113:MET:HA	2.03	0.40
1:G:166:GLU:HB2	1:G:328:GLY:HA3	2.02	0.40
1:E:157:GLU:HG2	1:E:337:ALA:HA	2.03	0.40
1:B:313:ARG:HA	1:B:337:ALA:H	1.87	0.40
1:A:268:GLN:HB3	1:A:269:LYS:H	1.65	0.40
1:G:300:THR:C	1:G:302:LYS:HG2	2.42	0.40
1:B:110:GLU:OE2	1:B:306:LEU:N	2.54	0.40
1:G:313:ARG:HA	1:G:336:ALA:HA	2.04	0.40
1:C:191:ALA:O	1:C:192:ARG:C	2.60	0.40
1:F:110:GLU:OE2	1:F:195:LEU:HD13	2.21	0.40
1:B:249:GLU:O	1:B:287:ASN:HA	2.21	0.40
1:F:131:ALA:C	1:F:133:ALA:N	2.75	0.40
1:G:150:SER:HB2	1:A:154:GLU:CD	2.42	0.40
1:F:325:TYR:CG	1:F:326:ALA:N	2.90	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	244/345 (71%)	180 (74%)	42 (17%)	22 (9%)	1	17
1	B	244/345 (71%)	183 (75%)	46 (19%)	15 (6%)	2	26
1	C	244/345 (71%)	183 (75%)	38 (16%)	23 (9%)	1	16
1	D	244/345 (71%)	179 (73%)	38 (16%)	27 (11%)	0	11
1	E	244/345 (71%)	186 (76%)	44 (18%)	14 (6%)	2	28
1	F	244/345 (71%)	179 (73%)	47 (19%)	18 (7%)	1	21
1	G	244/345 (71%)	186 (76%)	42 (17%)	16 (7%)	1	24
All	All	1708/2415 (71%)	1276 (75%)	297 (17%)	135 (8%)	2	19

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	240	ARG
1	G	302	LYS
1	A	127	GLY
1	A	239	ILE
1	A	283	VAL
1	A	336	ALA
1	B	137	ALA
1	B	157	GLU
1	B	239	ILE
1	B	283	VAL
1	B	336	ALA
1	C	126	LEU
1	C	138	VAL
1	C	145	LEU
1	C	148	VAL
1	C	194	ALA
1	C	239	ILE
1	C	283	VAL

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Mol	Chain	Res	Type
1	C	299	GLY
1	C	336	ALA
1	D	127	GLY
1	D	239	ILE
1	E	157	GLU
1	E	240	ARG
1	E	283	VAL
1	E	336	ALA
1	F	126	LEU
1	F	145	LEU
1	F	148	VAL
1	F	194	ALA
1	F	239	ILE
1	F	283	VAL
1	F	336	ALA
1	G	126	LEU
1	G	158	GLY
1	G	282	LYS
1	G	336	ALA
1	A	135	ASP
1	A	142	ILE
1	A	143	ALA
1	A	158	GLY
1	A	228	TYR
1	A	240	ARG
1	A	299	GLY
1	A	339	ALA
1	B	158	GLY
1	B	299	GLY
1	C	134	ALA
1	C	135	ASP
1	C	157	GLU
1	C	228	TYR
1	C	268	GLN
1	C	301	VAL
1	D	133	ALA
1	D	139	LEU
1	D	142	ILE
1	D	228	TYR
1	D	282	LYS
1	D	336	ALA
1	E	158	GLY

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Mol	Chain	Res	Type
1	E	228	TYR
1	E	299	GLY
1	F	157	GLU
1	F	158	GLY
1	F	228	TYR
1	G	137	ALA
1	G	198	ASN
1	G	212	ASP
1	G	268	GLN
1	A	146	CYS
1	A	198	ASN
1	A	212	ASP
1	A	268	GLN
1	A	282	LYS
1	B	161	THR
1	B	198	ASN
1	B	268	GLN
1	C	158	GLY
1	C	198	ASN
1	C	282	LYS
1	D	137	ALA
1	D	212	ASP
1	D	268	GLN
1	D	283	VAL
1	E	198	ASN
1	E	212	ASP
1	E	268	GLN
1	E	282	LYS
1	E	340	VAL
1	F	142	ILE
1	F	198	ASN
1	F	241	ASN
1	F	268	GLN
1	F	282	LYS
1	F	299	GLY
1	F	340	VAL
1	G	191	ALA
1	G	283	VAL
1	G	299	GLY
1	A	208	TYR
1	A	340	VAL
1	B	208	TYR

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Mol	Chain	Res	Type
1	C	142	ILE
1	C	212	ASP
1	C	340	VAL
1	D	135	ASP
1	D	143	ALA
1	D	198	ASN
1	D	340	VAL
1	G	160	GLY
1	G	208	TYR
1	A	160	GLY
1	A	191	ALA
1	B	138	VAL
1	B	212	ASP
1	B	228	TYR
1	B	340	VAL
1	C	208	TYR
1	D	131	ALA
1	D	146	CYS
1	D	158	GLY
1	D	160	GLY
1	D	191	ALA
1	D	299	GLY
1	D	306	LEU
1	E	191	ALA
1	A	148	VAL
1	D	126	LEU
1	D	208	TYR
1	E	160	GLY
1	G	340	VAL
1	C	160	GLY
1	F	160	GLY
1	D	148	VAL
1	D	334	PRO

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 PDB entries followed by that with respect to all EM entries.

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	184/261 (70%)	160 (87%)	24 (13%)	5	28
1	B	184/261 (70%)	165 (90%)	19 (10%)	9	37
1	C	184/261 (70%)	163 (89%)	21 (11%)	7	33
1	D	184/261 (70%)	169 (92%)	15 (8%)	14	49
1	E	184/261 (70%)	170 (92%)	14 (8%)	16	53
1	F	184/261 (70%)	167 (91%)	17 (9%)	11	43
1	G	184/261 (70%)	168 (91%)	16 (9%)	13	45
All	All	1288/1827 (70%)	1162 (90%)	126 (10%)	14	39

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	117	ASP
1	G	119	ARG
1	G	120	SER
1	G	122	TYR
1	G	150	SER
1	G	197	LYS
1	G	198	ASN
1	G	282	LYS
1	G	295	ARG
1	G	298	VAL
1	G	301	VAL
1	G	308	LEU
1	G	310	ARG
1	G	315	ASN
1	G	342	PHE
1	G	343	LYS
1	A	117	ASP
1	A	118	VAL
1	A	119	ARG
1	A	121	GLU
1	A	122	TYR
1	A	123	THR
1	A	139	LEU
1	A	142	ILE
1	A	197	LYS
1	A	204	ASP
1	A	231	LEU
1	A	232	ILE
1	A	240	ARG

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Mol	Chain	Res	Type
1	A	282	LYS
1	A	293	MET
1	A	295	ARG
1	A	304	ARG
1	A	308	LEU
1	A	310	ARG
1	A	315	ASN
1	A	340	VAL
1	A	341	VAL
1	A	342	PHE
1	A	343	LYS
1	B	119	ARG
1	B	122	TYR
1	B	135	ASP
1	B	197	LYS
1	B	198	ASN
1	B	204	ASP
1	B	240	ARG
1	B	282	LYS
1	B	293	MET
1	B	295	ARG
1	B	298	VAL
1	B	301	VAL
1	B	302	LYS
1	B	308	LEU
1	B	310	ARG
1	B	315	ASN
1	B	340	VAL
1	B	342	PHE
1	B	343	LYS
1	C	119	ARG
1	C	122	TYR
1	C	126	LEU
1	C	130	LEU
1	C	148	VAL
1	C	196	THR
1	C	197	LYS
1	C	198	ASN
1	C	238	SER
1	C	243	MET
1	C	282	LYS
1	C	293	MET

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Mol	Chain	Res	Type
1	C	295	ARG
1	C	302	LYS
1	C	308	LEU
1	C	310	ARG
1	C	315	ASN
1	C	340	VAL
1	C	341	VAL
1	C	342	PHE
1	C	343	LYS
1	D	119	ARG
1	D	122	TYR
1	D	126	LEU
1	D	196	THR
1	D	197	LYS
1	D	198	ASN
1	D	240	ARG
1	D	282	LYS
1	D	295	ARG
1	D	302	LYS
1	D	308	LEU
1	D	310	ARG
1	D	315	ASN
1	D	342	PHE
1	D	343	LYS
1	E	119	ARG
1	E	122	TYR
1	E	197	LYS
1	E	198	ASN
1	E	240	ARG
1	E	282	LYS
1	E	295	ARG
1	E	302	LYS
1	E	308	LEU
1	E	310	ARG
1	E	315	ASN
1	E	340	VAL
1	E	342	PHE
1	E	343	LYS
1	F	119	ARG
1	F	122	TYR
1	F	126	LEU
1	F	135	ASP

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Mol	Chain	Res	Type
1	F	197	LYS
1	F	198	ASN
1	F	243	MET
1	F	282	LYS
1	F	293	MET
1	F	295	ARG
1	F	301	VAL
1	F	308	LEU
1	F	310	ARG
1	F	315	ASN
1	F	340	VAL
1	F	342	PHE
1	F	343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	153	ASN
1	G	224	ASN
1	G	287	ASN
1	G	315	ASN
1	G	320	GLN
1	A	153	ASN
1	A	224	ASN
1	A	287	ASN
1	A	315	ASN
1	A	320	GLN
1	B	153	ASN
1	B	287	ASN
1	B	315	ASN
1	B	320	GLN
1	B	329	HIS
1	C	153	ASN
1	C	287	ASN
1	C	315	ASN
1	C	320	GLN
1	D	153	ASN
1	D	155	ASN
1	D	224	ASN
1	D	287	ASN
1	D	315	ASN
1	D	317	GLN

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Mol	Chain	Res	Type
1	D	320	GLN
1	E	153	ASN
1	E	287	ASN
1	E	315	ASN
1	E	317	GLN
1	E	320	GLN
1	F	153	ASN
1	F	224	ASN
1	F	287	ASN
1	F	315	ASN
1	F	317	GLN
1	F	320	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.