



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 28, 2017 – 11:28 PM EDT

PDB ID : 5OGW
EMDB ID: : EMD-3805
Title : Cryo-EM structure of jasplakinolide-stabilized malaria parasite F-actin at near-atomic resolution
Authors : Pospich, S.; Kumpula, E.-P.; von der Ecken, J.; Vahokoski, J.; Kursula, I.; Raunser, S.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

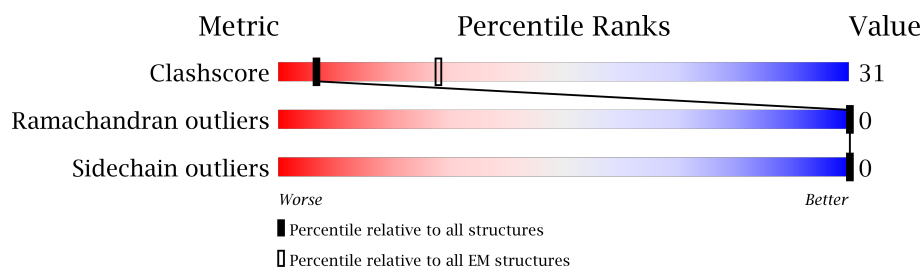
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	378	56% 42% .
1	B	378	57% 41% .
1	C	378	57% 41% .
1	D	378	57% 41% .
1	E	378	56% 42% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14736 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 Actin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2891	1829	489	557	16		
1	B	370	Total	C	N	O	S	0	0
			2891	1829	489	557	16		
1	C	370	Total	C	N	O	S	0	0
			2891	1829	489	557	16		
1	D	370	Total	C	N	O	S	0	0
			2891	1829	489	557	16		
1	E	370	Total	C	N	O	S	0	0
			2891	1829	489	557	16		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P86287
A	2	ALA	-	expression tag	UNP P86287
B	1	GLY	-	expression tag	UNP P86287
B	2	ALA	-	expression tag	UNP P86287
C	1	GLY	-	expression tag	UNP P86287
C	2	ALA	-	expression tag	UNP P86287
D	1	GLY	-	expression tag	UNP P86287
D	2	ALA	-	expression tag	UNP P86287
E	1	GLY	-	expression tag	UNP P86287
E	2	ALA	-	expression tag	UNP P86287

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

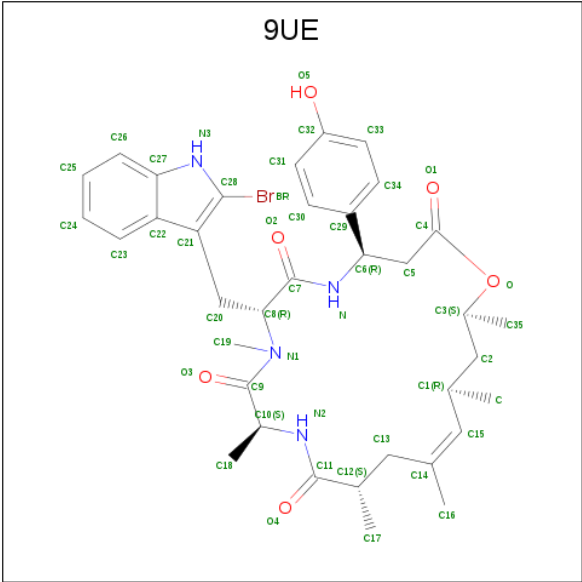


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total Mg 1 1	0
3	A	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0

- Molecule 4 is Jasplakinolide (three-letter code: 9UE) (formula: $C_{36}H_{45}BrN_4O_6$).

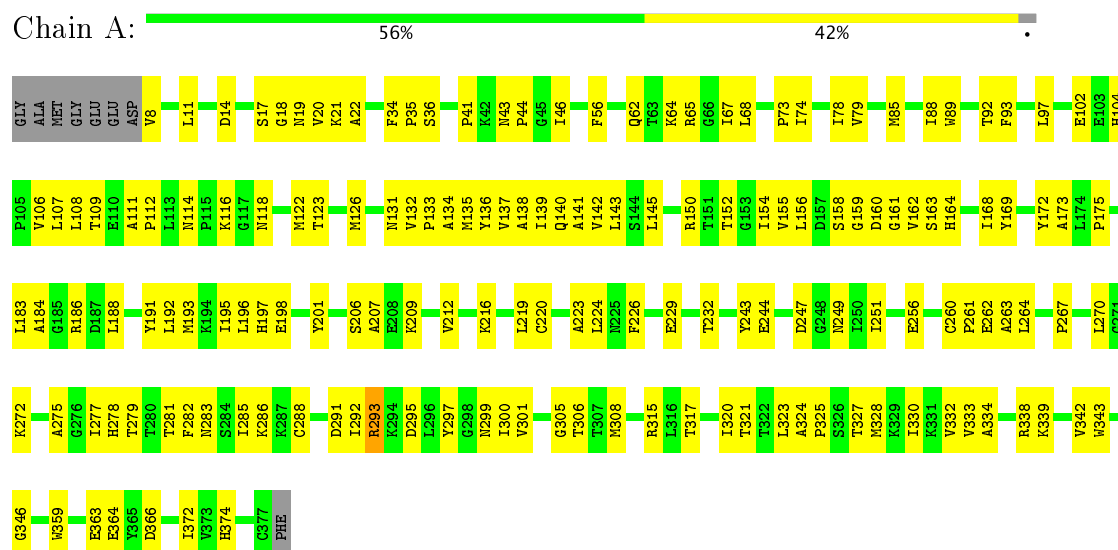


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	Br	C	N	O	0
			47	1	36	4	6	
4	C	1	Total	Br	C	N	O	0
			47	1	36	4	6	
4	E	1	Total	Br	C	N	O	0
			47	1	36	4	6	

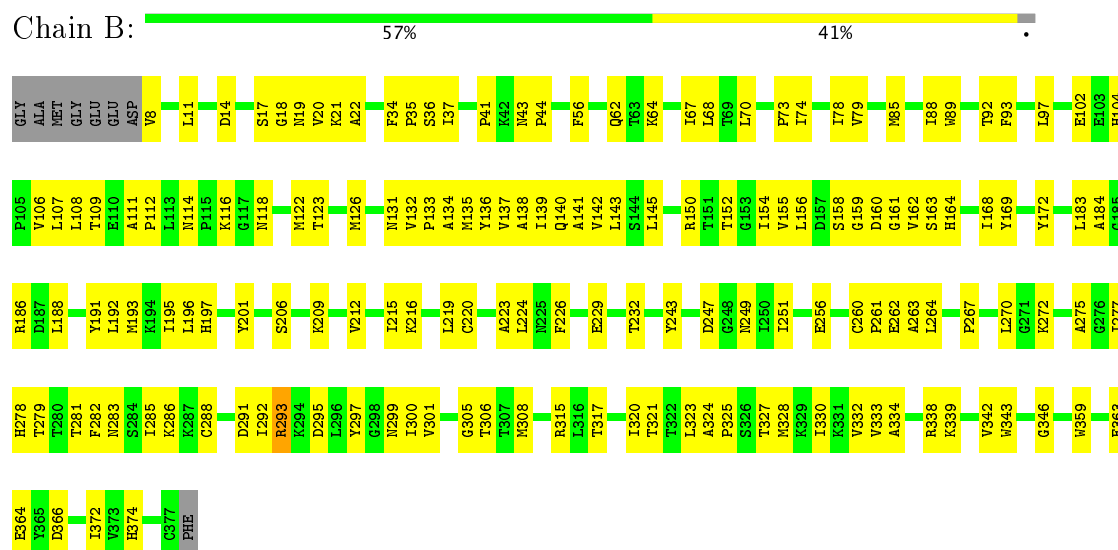
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Actin-1

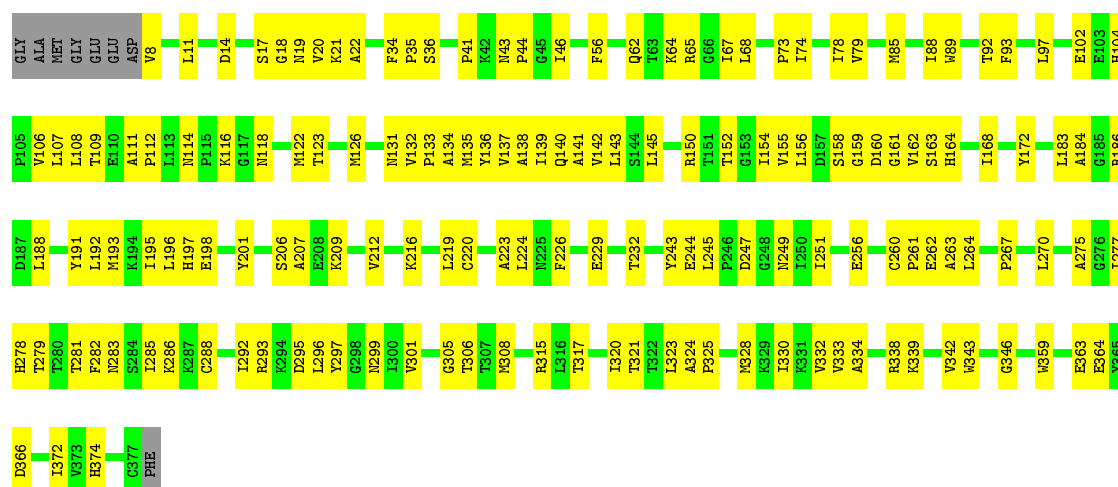


• Molecule 1: Actin-1

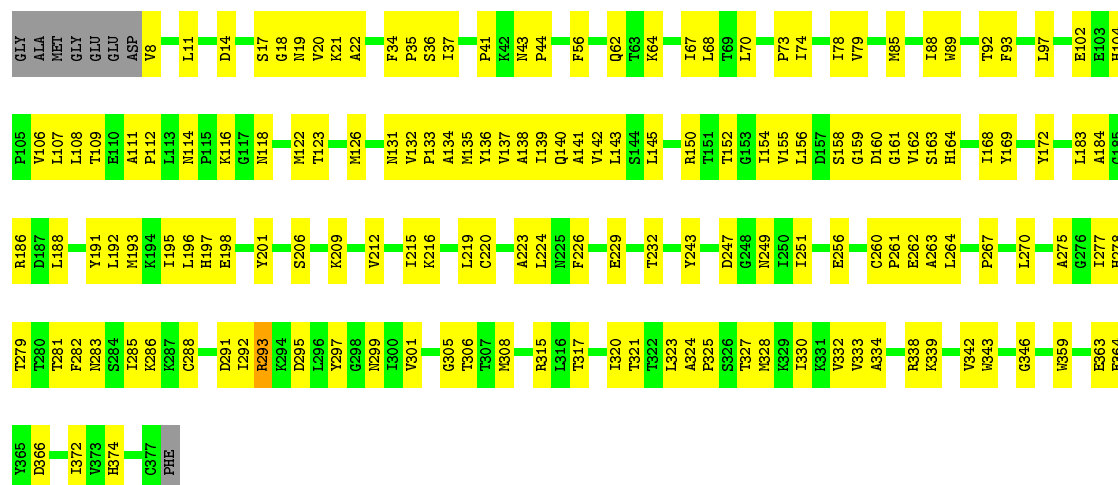


• Molecule 1: Actin-1

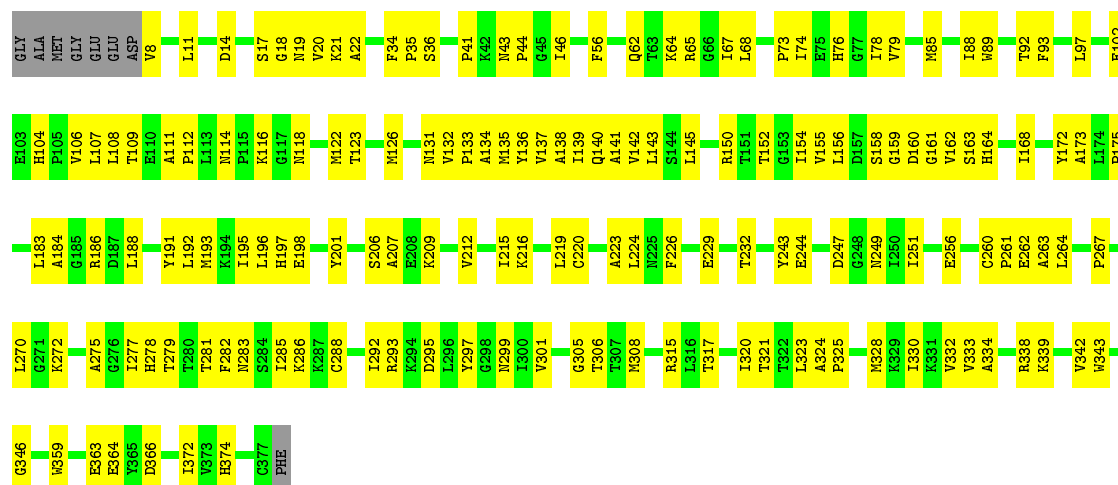




• Molecule 1: Actin-1



• Molecule 1: Actin-1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140716	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	110	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 9UE, ADP

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	0.53	0/2952	0.65	1/3996 (0.0%)
1	B	0.52	0/2952	0.65	1/3996 (0.0%)
1	C	0.52	0/2952	0.64	0/3996
1	D	0.53	0/2952	0.65	1/3996 (0.0%)
1	E	0.53	0/2952	0.64	0/3996
All	All	0.52	0/14760	0.64	3/19980 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	293	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	D	293	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2891	0	2867	194	0
1	B	2891	0	2867	187	0
1	C	2891	0	2867	184	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2891	0	2867	181	0
1	E	2891	0	2867	185	0
2	A	27	0	12	1	0
2	B	27	0	12	2	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	47	0	0	0	0
4	C	47	0	0	4	0
4	E	47	0	0	0	0
All	All	14736	0	14395	899	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 31.

All (899) 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:D:286:LYS:HA	1:D:293:ARG:HH12	1.22	1.04
1:B:286:LYS:HA	1:B:293:ARG:HH12	1.23	1.02
1:C:286:LYS:HA	1:C:293:ARG:HH12	1.23	1.01
1:B:183:LEU:HD11	1:B:267:PRO:HB3	1.43	1.01
1:E:286:LYS:HA	1:E:293:ARG:HH12	1.23	1.00
1:A:183:LEU:HD11	1:A:267:PRO:HB3	1.44	1.00
1:C:183:LEU:HD11	1:C:267:PRO:HB3	1.43	0.99
1:A:286:LYS:HA	1:A:293:ARG:HH12	1.23	0.99
1:D:183:LEU:HD11	1:D:267:PRO:HB3	1.43	0.97
1:E:183:LEU:HD11	1:E:267:PRO:HB3	1.43	0.97
1:C:112:PRO:HD3	1:C:139:ILE:HG23	1.52	0.91
1:A:183:LEU:HD22	1:A:270:LEU:HD12	1.53	0.91
1:C:183:LEU:HD22	1:C:270:LEU:HD12	1.52	0.91
1:A:112:PRO:HD3	1:A:139:ILE:HG23	1.53	0.90
1:B:183:LEU:HD22	1:B:270:LEU:HD12	1.52	0.90
1:D:183:LEU:HD22	1:D:270:LEU:HD12	1.52	0.90
1:D:112:PRO:HD3	1:D:139:ILE:HG23	1.53	0.90
1:E:183:LEU:HD22	1:E:270:LEU:HD12	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PRO:HD3	1:B:139:ILE:HG23	1.53	0.89
1:E:112:PRO:HD3	1:E:139:ILE:HG23	1.54	0.89
1:C:14:ASP:OD1	1:C:109:THR:OG1	1.95	0.85
1:A:14:ASP:OD1	1:A:109:THR:OG1	1.95	0.85
1:B:14:ASP:OD1	1:B:109:THR:OG1	1.95	0.84
1:D:14:ASP:OD1	1:D:109:THR:OG1	1.95	0.84
1:C:201:TYR:HE1	4:C:403:9UE:C35	1.91	0.83
1:E:14:ASP:OD1	1:E:109:THR:OG1	1.95	0.82
1:B:154:ILE:HD11	1:B:285:ILE:HG13	1.64	0.79
1:A:154:ILE:HD11	1:A:285:ILE:HG13	1.64	0.79
1:B:219:LEU:HD11	1:B:243:TYR:HB2	1.64	0.79
1:A:219:LEU:HD11	1:A:243:TYR:HB2	1.65	0.78
1:A:169:TYR:HD2	1:C:67:ILE:HD11	1.49	0.78
1:B:275:ALA:HB1	1:B:279:THR:OG1	1.84	0.77
1:C:219:LEU:HD11	1:C:243:TYR:HB2	1.66	0.77
1:E:154:ILE:HD11	1:E:285:ILE:HG13	1.64	0.77
1:C:154:ILE:HD11	1:C:285:ILE:HG13	1.65	0.77
1:E:275:ALA:HB1	1:E:279:THR:OG1	1.84	0.77
1:A:158:SER:OG	1:A:306:THR:HB	1.84	0.77
1:A:275:ALA:HB1	1:A:279:THR:OG1	1.85	0.77
1:D:154:ILE:HD11	1:D:285:ILE:HG13	1.65	0.77
1:C:158:SER:OG	1:C:306:THR:HB	1.84	0.77
1:D:183:LEU:HD22	1:D:270:LEU:CD1	2.15	0.77
1:B:158:SER:OG	1:B:306:THR:HB	1.84	0.76
1:D:158:SER:OG	1:D:306:THR:HB	1.84	0.76
1:D:188:LEU:HD11	1:D:264:LEU:HD21	1.67	0.76
1:E:17:SER:O	1:E:160:ASP:HB2	1.86	0.76
1:E:141:ALA:HB1	1:E:155:VAL:HG23	1.66	0.76
1:E:219:LEU:HD11	1:E:243:TYR:HB2	1.66	0.76
1:E:183:LEU:HD22	1:E:270:LEU:CD1	2.15	0.76
1:D:275:ALA:HB1	1:D:279:THR:OG1	1.86	0.76
1:A:141:ALA:HB1	1:A:155:VAL:HG23	1.67	0.76
1:D:219:LEU:HD11	1:D:243:TYR:HB2	1.65	0.76
1:B:141:ALA:HB1	1:B:155:VAL:HG23	1.68	0.76
1:B:183:LEU:HD22	1:B:270:LEU:CD1	2.15	0.76
1:C:201:TYR:CE2	1:C:251:ILE:HG23	2.21	0.75
1:D:141:ALA:HB1	1:D:155:VAL:HG23	1.67	0.75
1:D:17:SER:O	1:D:160:ASP:HB2	1.86	0.75
1:E:158:SER:OG	1:E:306:THR:HB	1.85	0.75
1:C:183:LEU:HD22	1:C:270:LEU:CD1	2.15	0.75
1:A:247:ASP:OD2	1:A:249:ASN:ND2	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ALA:HB1	1:C:155:VAL:HG23	1.67	0.75
1:C:17:SER:OG	1:C:161:GLY:N	2.20	0.75
1:C:247:ASP:OD2	1:C:249:ASN:ND2	2.20	0.75
1:C:275:ALA:HB1	1:C:279:THR:OG1	1.85	0.75
1:E:247:ASP:OD2	1:E:249:ASN:ND2	2.20	0.75
1:A:201:TYR:CE2	1:A:251:ILE:HG23	2.22	0.75
1:A:17:SER:O	1:A:160:ASP:HB2	1.85	0.74
1:E:201:TYR:CE2	1:E:251:ILE:HG23	2.22	0.74
1:C:17:SER:O	1:C:160:ASP:HB2	1.86	0.74
1:E:188:LEU:HD11	1:E:264:LEU:HD21	1.69	0.74
1:C:188:LEU:HD11	1:C:264:LEU:HD21	1.67	0.74
1:A:89:TRP:O	1:A:92:THR:OG1	2.05	0.74
1:D:169:TYR:HD2	1:E:67:ILE:HD11	1.52	0.74
1:A:188:LEU:HD11	1:A:264:LEU:HD21	1.68	0.74
1:B:112:PRO:HD2	1:B:164:HIS:CE1	2.23	0.74
1:A:67:ILE:HD11	1:B:169:TYR:HD2	1.53	0.74
1:E:17:SER:OG	1:E:161:GLY:N	2.21	0.74
1:A:183:LEU:HD22	1:A:270:LEU:CD1	2.16	0.74
1:B:188:LEU:HD11	1:B:264:LEU:HD21	1.69	0.74
1:B:247:ASP:OD2	1:B:249:ASN:ND2	2.21	0.74
1:D:17:SER:OG	1:D:161:GLY:N	2.21	0.74
1:D:247:ASP:OD2	1:D:249:ASN:ND2	2.21	0.74
1:B:17:SER:O	1:B:160:ASP:HB2	1.87	0.73
1:C:89:TRP:O	1:C:92:THR:OG1	2.04	0.73
1:D:112:PRO:HD2	1:D:164:HIS:CE1	2.23	0.73
1:D:201:TYR:CE2	1:D:251:ILE:HG23	2.23	0.73
1:B:201:TYR:CE2	1:B:251:ILE:HG23	2.24	0.73
1:E:112:PRO:HD2	1:E:164:HIS:CE1	2.23	0.73
1:A:112:PRO:HD2	1:A:164:HIS:CE1	2.24	0.73
1:B:17:SER:OG	1:B:161:GLY:N	2.22	0.73
1:A:17:SER:OG	1:A:161:GLY:N	2.21	0.73
1:D:159:GLY:O	1:D:184:ALA:HB1	1.89	0.73
1:E:159:GLY:O	1:E:184:ALA:HB1	1.89	0.72
1:A:159:GLY:O	1:A:184:ALA:HB1	1.89	0.72
1:B:159:GLY:O	1:B:184:ALA:HB1	1.89	0.72
1:C:159:GLY:O	1:C:184:ALA:HB1	1.90	0.72
1:C:112:PRO:HD2	1:C:164:HIS:CE1	2.24	0.72
1:B:116:LYS:HD2	1:D:198:GLU:HG2	1.72	0.72
1:E:21:LYS:NZ	1:E:339:LYS:O	2.24	0.71
1:A:260:CYS:HB3	1:A:261:PRO:HD3	1.72	0.71
1:D:78:ILE:HA	1:D:118:ASN:HD21	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TYR:CE1	4:C:403:9UE:C35	2.74	0.71
1:E:89:TRP:O	1:E:92:THR:OG1	2.05	0.71
1:B:111:ALA:O	1:B:114:ASN:HB2	1.91	0.70
1:E:111:ALA:O	1:E:114:ASN:HB2	1.91	0.70
1:B:78:ILE:HA	1:B:118:ASN:HD21	1.56	0.70
1:E:78:ILE:HA	1:E:118:ASN:HD21	1.56	0.70
1:D:111:ALA:O	1:D:114:ASN:HB2	1.92	0.70
1:A:111:ALA:O	1:A:114:ASN:HB2	1.92	0.70
1:D:155:VAL:HG12	1:D:301:VAL:CG2	2.22	0.70
1:C:78:ILE:HA	1:C:118:ASN:HD21	1.54	0.70
1:A:195:ILE:CG2	1:A:256:GLU:HG3	2.22	0.70
1:C:195:ILE:CG2	1:C:256:GLU:HG3	2.22	0.70
1:D:195:ILE:CG2	1:D:256:GLU:HG3	2.21	0.70
1:B:195:ILE:CG2	1:B:256:GLU:HG3	2.22	0.70
1:C:260:CYS:HB3	1:C:261:PRO:HD3	1.73	0.70
1:D:183:LEU:CD1	1:D:267:PRO:HB3	2.21	0.70
1:E:260:CYS:HB3	1:E:261:PRO:HD3	1.73	0.70
1:C:109:THR:CG2	1:C:140:GLN:HG2	2.22	0.70
1:A:198:GLU:HG2	1:D:116:LYS:HD2	1.73	0.70
1:B:21:LYS:NZ	1:B:339:LYS:O	2.24	0.69
1:C:56:PHE:CE2	1:C:64:LYS:HD2	2.26	0.69
1:D:109:THR:CG2	1:D:140:GLN:HG2	2.22	0.69
1:C:21:LYS:NZ	1:C:339:LYS:O	2.25	0.69
1:D:56:PHE:CE2	1:D:64:LYS:HD2	2.27	0.69
1:E:155:VAL:HG12	1:E:301:VAL:CG2	2.23	0.69
1:E:56:PHE:CE2	1:E:64:LYS:HD2	2.27	0.69
1:E:183:LEU:CD1	1:E:267:PRO:HB3	2.21	0.69
1:B:183:LEU:CD1	1:B:267:PRO:HB3	2.21	0.69
1:C:111:ALA:O	1:C:114:ASN:HB2	1.93	0.69
1:D:21:LYS:NZ	1:D:339:LYS:O	2.25	0.69
1:C:108:LEU:O	1:C:137:VAL:HA	1.93	0.69
1:D:89:TRP:O	1:D:92:THR:OG1	2.05	0.69
1:D:260:CYS:HB3	1:D:261:PRO:HD3	1.73	0.69
1:E:108:LEU:O	1:E:137:VAL:HA	1.92	0.69
1:A:155:VAL:HG12	1:A:301:VAL:CG2	2.22	0.69
1:A:78:ILE:HA	1:A:118:ASN:HD21	1.57	0.69
1:E:195:ILE:CG2	1:E:256:GLU:HG3	2.23	0.69
1:A:21:LYS:NZ	1:A:339:LYS:O	2.25	0.69
1:B:108:LEU:O	1:B:137:VAL:HA	1.93	0.68
1:B:56:PHE:CE2	1:B:64:LYS:HD2	2.28	0.68
1:C:35:PRO:HG3	1:C:62:GLN:OE1	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:LEU:HD11	1:D:264:LEU:CD2	2.23	0.68
1:E:109:THR:CG2	1:E:140:GLN:HG2	2.23	0.68
1:A:188:LEU:HD11	1:A:264:LEU:CD2	2.24	0.68
1:D:108:LEU:O	1:D:137:VAL:HA	1.93	0.68
1:B:260:CYS:HB3	1:B:261:PRO:HD3	1.73	0.68
1:D:155:VAL:HG12	1:D:301:VAL:HG21	1.76	0.68
1:A:183:LEU:CD1	1:A:267:PRO:HB3	2.21	0.68
1:A:35:PRO:HG3	1:A:62:GLN:OE1	1.94	0.68
1:C:155:VAL:HG12	1:C:301:VAL:CG2	2.23	0.68
1:A:56:PHE:CE2	1:A:64:LYS:HD2	2.28	0.68
1:A:109:THR:CG2	1:A:140:GLN:HG2	2.24	0.68
1:B:35:PRO:HG3	1:B:62:GLN:OE1	1.93	0.68
1:C:188:LEU:HD11	1:C:264:LEU:CD2	2.23	0.68
1:C:183:LEU:CD1	1:C:267:PRO:HB3	2.22	0.68
1:D:35:PRO:HG3	1:D:62:GLN:OE1	1.93	0.68
1:A:108:LEU:O	1:A:137:VAL:HA	1.92	0.68
1:B:155:VAL:HG12	1:B:301:VAL:CG2	2.23	0.68
1:B:89:TRP:O	1:B:92:THR:OG1	2.04	0.67
1:E:188:LEU:HD11	1:E:264:LEU:CD2	2.24	0.67
1:B:109:THR:CG2	1:B:140:GLN:HG2	2.24	0.67
1:B:188:LEU:HD11	1:B:264:LEU:CD2	2.24	0.67
1:E:35:PRO:HG3	1:E:62:GLN:OE1	1.95	0.67
1:A:111:ALA:HB1	1:A:164:HIS:HE1	1.59	0.66
1:A:198:GLU:CG	1:D:116:LYS:HD2	2.25	0.66
1:E:155:VAL:HG12	1:E:301:VAL:HG21	1.78	0.66
1:A:155:VAL:HG12	1:A:301:VAL:HG21	1.76	0.66
1:C:111:ALA:HB1	1:C:164:HIS:HE1	1.61	0.66
1:D:111:ALA:HB1	1:D:164:HIS:HE1	1.60	0.66
1:B:111:ALA:HB1	1:B:164:HIS:HE1	1.62	0.65
1:E:154:ILE:HD11	1:E:285:ILE:CG1	2.27	0.65
1:C:152:THR:HG21	1:C:295:ASP:HB3	1.79	0.65
1:B:155:VAL:HG12	1:B:301:VAL:HG21	1.78	0.65
1:D:154:ILE:HD11	1:D:285:ILE:CG1	2.26	0.65
1:E:22:ALA:HB1	1:E:97:LEU:HD11	1.79	0.65
1:E:111:ALA:HB1	1:E:164:HIS:HE1	1.61	0.65
1:C:155:VAL:HG12	1:C:301:VAL:HG21	1.77	0.65
1:C:41:PRO:HA	1:C:68:LEU:HD23	1.79	0.65
1:D:142:VAL:HG12	1:D:168:ILE:HD11	1.79	0.64
1:D:160:ASP:OD1	2:D:401:ADP:H4'	1.97	0.64
1:A:152:THR:HG21	1:A:295:ASP:HB3	1.80	0.64
1:C:154:ILE:HD11	1:C:285:ILE:CG1	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HD11	1:A:285:ILE:CG1	2.27	0.64
1:B:112:PRO:CD	1:B:139:ILE:HG23	2.27	0.64
1:A:41:PRO:HA	1:A:68:LEU:HD23	1.80	0.64
1:B:154:ILE:HD11	1:B:285:ILE:CG1	2.27	0.64
1:B:152:THR:HG21	1:B:295:ASP:HB3	1.80	0.64
1:E:56:PHE:HD2	1:E:68:LEU:HD11	1.63	0.64
1:B:56:PHE:HD2	1:B:68:LEU:HD11	1.62	0.64
1:A:22:ALA:HB1	1:A:97:LEU:HD11	1.79	0.64
1:B:142:VAL:HG12	1:B:168:ILE:HD11	1.78	0.64
1:D:152:THR:HG21	1:D:295:ASP:HB3	1.79	0.64
1:D:22:ALA:HB1	1:D:97:LEU:HD11	1.80	0.64
1:A:160:ASP:OD1	2:A:401:ADP:H4'	1.96	0.64
1:E:160:ASP:OD1	2:E:401:ADP:H4'	1.98	0.64
1:B:41:PRO:HA	1:B:68:LEU:HD23	1.80	0.64
1:A:142:VAL:HG12	1:A:168:ILE:HD11	1.79	0.64
1:A:320:ILE:HG22	1:A:330:ILE:HD13	1.80	0.64
1:B:116:LYS:HD2	1:D:198:GLU:CG	2.27	0.64
1:B:22:ALA:HB1	1:B:97:LEU:HD11	1.79	0.64
1:D:41:PRO:HA	1:D:68:LEU:HD23	1.80	0.64
1:A:111:ALA:HB1	1:A:164:HIS:CE1	2.33	0.63
1:C:22:ALA:HB1	1:C:97:LEU:HD11	1.80	0.63
1:E:320:ILE:HG22	1:E:330:ILE:HD13	1.80	0.63
1:E:156:LEU:HD22	1:E:281:THR:OG1	1.99	0.63
1:E:142:VAL:HG12	1:E:168:ILE:HD11	1.79	0.63
1:E:64:LYS:O	1:E:64:LYS:HG3	1.98	0.63
1:E:41:PRO:HA	1:E:68:LEU:HD23	1.79	0.63
1:A:156:LEU:HD22	1:A:281:THR:OG1	1.99	0.63
1:B:320:ILE:HG22	1:B:330:ILE:HD13	1.81	0.63
1:E:141:ALA:HB1	1:E:155:VAL:CG2	2.29	0.63
1:D:141:ALA:HB1	1:D:155:VAL:CG2	2.29	0.63
1:D:56:PHE:HD2	1:D:68:LEU:HD11	1.64	0.62
1:A:141:ALA:HB1	1:A:155:VAL:CG2	2.28	0.62
1:B:156:LEU:HD22	1:B:281:THR:OG1	1.98	0.62
1:C:156:LEU:HD22	1:C:281:THR:OG1	1.99	0.62
1:C:320:ILE:HG22	1:C:330:ILE:HD13	1.81	0.62
1:A:142:VAL:HG11	1:C:46:ILE:HD13	1.80	0.62
1:C:160:ASP:OD1	2:C:401:ADP:H4'	1.98	0.62
1:E:152:THR:HG21	1:E:295:ASP:HB3	1.80	0.62
1:A:74:ILE:HD11	1:A:85:MET:CE	2.30	0.62
1:B:160:ASP:OD1	2:B:401:ADP:H4'	1.98	0.62
1:B:74:ILE:HD11	1:B:85:MET:CE	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:HD2	1:C:68:LEU:HD11	1.64	0.62
1:C:142:VAL:HG12	1:C:168:ILE:HD11	1.80	0.62
1:A:116:LYS:HD2	1:E:198:GLU:HG2	1.82	0.62
1:C:141:ALA:HB1	1:C:155:VAL:CG2	2.29	0.62
1:D:156:LEU:HD22	1:D:281:THR:OG1	2.00	0.62
1:D:320:ILE:HG22	1:D:330:ILE:HD13	1.82	0.62
1:A:64:LYS:HG3	1:A:64:LYS:O	1.99	0.62
1:C:301:VAL:HG23	1:C:301:VAL:O	2.00	0.62
1:C:64:LYS:O	1:C:64:LYS:HG3	2.00	0.62
1:C:102:GLU:HG2	1:C:131:ASN:HB3	1.83	0.61
1:B:14:ASP:OD2	1:B:342:VAL:HG12	2.00	0.61
1:C:112:PRO:CD	1:C:139:ILE:HG23	2.27	0.61
1:D:64:LYS:HG3	1:D:64:LYS:O	2.00	0.61
1:E:301:VAL:O	1:E:301:VAL:HG23	2.00	0.61
1:A:301:VAL:O	1:A:301:VAL:HG23	2.00	0.61
1:A:324:ALA:HB1	1:A:325:PRO:HD2	1.83	0.61
1:B:324:ALA:HB1	1:B:325:PRO:HD2	1.82	0.61
1:C:111:ALA:HB1	1:C:164:HIS:CE1	2.35	0.61
1:E:14:ASP:OD2	1:E:342:VAL:HG12	1.99	0.61
1:A:112:PRO:CD	1:A:139:ILE:HG23	2.27	0.61
1:A:56:PHE:HD2	1:A:68:LEU:HD11	1.64	0.61
1:C:74:ILE:HD11	1:C:85:MET:CE	2.30	0.61
1:E:324:ALA:HB1	1:E:325:PRO:HD2	1.82	0.61
1:D:14:ASP:OD2	1:D:342:VAL:HG12	2.00	0.61
1:E:288:CYS:HB3	1:E:292:ILE:HD11	1.83	0.61
1:B:141:ALA:HB1	1:B:155:VAL:CG2	2.30	0.61
1:C:324:ALA:HB1	1:C:325:PRO:HD2	1.83	0.61
1:A:14:ASP:OD2	1:A:342:VAL:HG12	2.00	0.61
1:B:64:LYS:HG3	1:B:64:LYS:O	2.00	0.61
1:A:102:GLU:HG2	1:A:131:ASN:HB3	1.83	0.61
1:D:288:CYS:HB3	1:D:292:ILE:HD11	1.83	0.61
1:E:74:ILE:HD11	1:E:85:MET:CE	2.31	0.61
1:B:108:LEU:HB2	1:B:137:VAL:HG12	1.82	0.61
1:D:301:VAL:HG23	1:D:301:VAL:O	2.01	0.61
1:D:324:ALA:HB1	1:D:325:PRO:HD2	1.83	0.61
1:C:108:LEU:HB2	1:C:137:VAL:HG12	1.82	0.61
1:D:111:ALA:HB1	1:D:164:HIS:CE1	2.35	0.61
1:A:288:CYS:HB3	1:A:292:ILE:HD11	1.83	0.60
1:C:288:CYS:HB3	1:C:292:ILE:HD11	1.83	0.60
1:C:14:ASP:OD2	1:C:342:VAL:HG12	2.00	0.60
1:E:111:ALA:HB1	1:E:164:HIS:CE1	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:PRO:CD	1:D:139:ILE:HG23	2.28	0.60
1:D:74:ILE:HD11	1:D:85:MET:CE	2.30	0.60
1:A:244:GLU:OE2	1:B:327:THR:HG21	2.01	0.60
1:E:108:LEU:HB2	1:E:137:VAL:HG12	1.82	0.60
1:C:206:SER:O	1:C:209:LYS:HG2	2.01	0.60
1:D:102:GLU:HG2	1:D:131:ASN:HB3	1.84	0.60
1:E:206:SER:O	1:E:209:LYS:HG2	2.01	0.60
1:E:332:VAL:O	1:E:332:VAL:HG23	2.02	0.60
1:B:206:SER:O	1:B:209:LYS:HG2	2.01	0.60
1:D:108:LEU:HB2	1:D:137:VAL:HG12	1.82	0.60
1:C:229:GLU:HA	1:C:232:THR:OG1	2.02	0.59
1:B:111:ALA:HB1	1:B:164:HIS:CE1	2.37	0.59
1:E:102:GLU:HG2	1:E:131:ASN:HB3	1.84	0.59
1:A:206:SER:O	1:A:209:LYS:HG2	2.02	0.59
1:D:109:THR:HG21	1:D:140:GLN:HG2	1.84	0.59
1:E:112:PRO:CD	1:E:139:ILE:HG23	2.28	0.59
1:B:288:CYS:HB3	1:B:292:ILE:HD11	1.84	0.59
1:A:192:LEU:HB2	1:A:260:CYS:SG	2.43	0.59
1:A:108:LEU:HB2	1:A:137:VAL:HG12	1.83	0.59
1:B:301:VAL:HG23	1:B:301:VAL:O	2.02	0.59
1:E:229:GLU:HA	1:E:232:THR:OG1	2.02	0.59
1:E:301:VAL:HG12	1:E:333:VAL:CG1	2.33	0.59
1:C:192:LEU:HB2	1:C:260:CYS:SG	2.43	0.59
1:D:229:GLU:HA	1:D:232:THR:OG1	2.02	0.59
1:A:278:HIS:HD2	1:A:323:LEU:HD11	1.68	0.59
1:B:325:PRO:HG2	1:B:328:MET:HE2	1.85	0.59
1:D:206:SER:O	1:D:209:LYS:HG2	2.02	0.59
1:A:229:GLU:HA	1:A:232:THR:OG1	2.02	0.58
1:B:229:GLU:HA	1:B:232:THR:OG1	2.02	0.58
1:C:245:LEU:HD11	4:C:403:9UE:C16	2.33	0.58
1:E:278:HIS:HD2	1:E:323:LEU:HD11	1.68	0.58
1:A:301:VAL:HG12	1:A:333:VAL:CG1	2.33	0.58
1:B:278:HIS:HD2	1:B:323:LEU:HD11	1.67	0.58
1:E:123:THR:O	1:E:126:MET:N	2.37	0.58
1:C:278:HIS:HD2	1:C:323:LEU:HD11	1.68	0.58
1:C:109:THR:HG21	1:C:140:GLN:HG2	1.84	0.58
1:E:192:LEU:HB2	1:E:260:CYS:SG	2.44	0.58
1:B:102:GLU:HG2	1:B:131:ASN:HB3	1.86	0.58
1:E:109:THR:HG21	1:E:140:GLN:HG2	1.85	0.58
1:D:278:HIS:HD2	1:D:323:LEU:HD11	1.68	0.58
1:B:192:LEU:HB2	1:B:260:CYS:SG	2.44	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:THR:O	1:D:126:MET:N	2.37	0.58
1:E:191:TYR:HB2	1:E:270:LEU:CD2	2.34	0.58
1:A:123:THR:O	1:A:126:MET:N	2.36	0.58
1:A:207:ALA:HB1	1:B:291:ASP:OD2	2.04	0.58
1:C:301:VAL:HG12	1:C:333:VAL:CG1	2.34	0.58
1:C:191:TYR:HB2	1:C:270:LEU:CD2	2.34	0.57
1:D:325:PRO:HG2	1:D:328:MET:HE2	1.86	0.57
1:D:191:TYR:HB2	1:D:270:LEU:CD2	2.34	0.57
1:B:123:THR:O	1:B:126:MET:N	2.37	0.57
1:D:192:LEU:HB2	1:D:260:CYS:SG	2.44	0.57
1:E:74:ILE:HD11	1:E:85:MET:HE1	1.86	0.57
1:A:191:TYR:HB2	1:A:270:LEU:CD2	2.34	0.57
1:D:74:ILE:HD11	1:D:85:MET:HE1	1.86	0.57
1:D:301:VAL:HG12	1:D:333:VAL:CG1	2.34	0.57
1:A:216:LYS:HA	1:A:220:CYS:SG	2.45	0.57
1:C:123:THR:O	1:C:126:MET:N	2.37	0.57
1:A:116:LYS:HD2	1:E:198:GLU:CG	2.34	0.57
1:A:332:VAL:O	1:A:332:VAL:HG23	2.04	0.57
1:B:191:TYR:HB2	1:B:270:LEU:CD2	2.34	0.57
1:D:327:THR:HG21	1:E:244:GLU:OE2	2.05	0.57
1:D:332:VAL:HG23	1:D:332:VAL:O	2.03	0.57
1:B:332:VAL:HG23	1:B:332:VAL:O	2.05	0.56
1:B:286:LYS:HA	1:B:293:ARG:NH1	2.07	0.56
1:D:172:TYR:CD2	1:E:67:ILE:HD13	2.41	0.56
1:C:74:ILE:HD11	1:C:85:MET:HE1	1.87	0.56
1:B:301:VAL:HG12	1:B:333:VAL:CG1	2.34	0.56
1:E:216:LYS:HA	1:E:220:CYS:SG	2.45	0.56
1:C:216:LYS:HA	1:C:220:CYS:SG	2.45	0.56
1:B:109:THR:HG21	1:B:140:GLN:HG2	1.86	0.56
1:B:216:LYS:HA	1:B:220:CYS:SG	2.46	0.56
1:D:216:LYS:HA	1:D:220:CYS:SG	2.46	0.55
1:C:160:ASP:O	1:C:184:ALA:HB3	2.06	0.55
1:D:160:ASP:O	1:D:184:ALA:HB3	2.06	0.55
1:E:160:ASP:O	1:E:184:ALA:HB3	2.06	0.55
1:A:109:THR:HG21	1:A:140:GLN:HG2	1.87	0.55
1:C:118:ASN:O	1:C:122:MET:HB2	2.07	0.55
1:C:138:ALA:CB	1:C:143:LEU:HD11	2.37	0.55
1:D:138:ALA:CB	1:D:143:LEU:HD11	2.37	0.55
1:A:160:ASP:O	1:A:184:ALA:HB3	2.06	0.55
1:B:74:ILE:HD11	1:B:85:MET:HE1	1.87	0.55
1:B:264:LEU:HB3	1:B:277:ILE:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD2	1:C:65:ARG:HG3	2.07	0.55
1:C:332:VAL:HG23	1:C:332:VAL:O	2.05	0.55
1:A:138:ALA:CB	1:A:143:LEU:HD11	2.37	0.55
1:B:138:ALA:CB	1:B:143:LEU:HD11	2.37	0.55
1:B:160:ASP:O	1:B:184:ALA:HB3	2.06	0.55
1:A:264:LEU:HB3	1:A:277:ILE:HD12	1.89	0.54
1:A:334:ALA:HB1	1:A:338:ARG:NH1	2.22	0.54
1:C:264:LEU:HB3	1:C:277:ILE:HD12	1.89	0.54
1:E:320:ILE:HG22	1:E:330:ILE:CD1	2.37	0.54
1:B:118:ASN:O	1:B:122:MET:HB2	2.07	0.54
1:E:138:ALA:CB	1:E:143:LEU:HD11	2.38	0.54
1:C:109:THR:HG22	1:C:140:GLN:HG2	1.89	0.54
1:C:78:ILE:HA	1:C:118:ASN:ND2	2.22	0.54
1:D:264:LEU:HB3	1:D:277:ILE:HD12	1.88	0.54
1:B:334:ALA:HB1	1:B:338:ARG:NH1	2.23	0.54
1:D:109:THR:HG22	1:D:140:GLN:HG2	1.88	0.54
1:E:325:PRO:HG2	1:E:328:MET:HE2	1.89	0.54
1:B:183:LEU:CD2	1:B:270:LEU:HD12	2.33	0.54
1:B:321:THR:OG1	1:B:330:ILE:HD12	2.08	0.54
1:A:109:THR:HG22	1:A:140:GLN:HG2	1.90	0.54
1:A:46:ILE:HD13	1:B:142:VAL:HG11	1.89	0.54
1:B:195:ILE:HG22	1:B:256:GLU:HG3	1.90	0.54
1:B:320:ILE:HG22	1:B:330:ILE:CD1	2.37	0.54
1:E:264:LEU:HB3	1:E:277:ILE:HD12	1.89	0.54
1:A:278:HIS:CD2	1:A:279:THR:HG23	2.43	0.54
1:A:321:THR:OG1	1:A:330:ILE:HD12	2.08	0.54
1:D:278:HIS:CD2	1:D:279:THR:HG23	2.43	0.54
1:C:198:GLU:HG2	1:E:116:LYS:HD2	1.89	0.54
1:D:118:ASN:O	1:D:122:MET:HB2	2.08	0.54
1:D:191:TYR:HB2	1:D:270:LEU:HD21	1.90	0.54
1:D:320:ILE:HG22	1:D:330:ILE:CD1	2.38	0.54
1:D:334:ALA:HB1	1:D:338:ARG:NH1	2.23	0.54
1:A:118:ASN:O	1:A:122:MET:HB2	2.07	0.53
1:A:320:ILE:HG22	1:A:330:ILE:CD1	2.37	0.53
1:A:74:ILE:HD11	1:A:79:VAL:HG22	1.89	0.53
1:C:334:ALA:HB1	1:C:338:ARG:NH1	2.23	0.53
1:E:118:ASN:O	1:E:122:MET:HB2	2.08	0.53
1:E:334:ALA:HB1	1:E:338:ARG:NH1	2.22	0.53
1:A:286:LYS:HA	1:A:293:ARG:NH1	2.08	0.53
1:A:74:ILE:HD11	1:A:85:MET:HE1	1.90	0.53
1:C:195:ILE:HG22	1:C:256:GLU:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:THR:OG1	1:C:330:ILE:HD12	2.08	0.53
1:C:325:PRO:HG2	1:C:328:MET:HE2	1.90	0.53
1:E:109:THR:HG22	1:E:140:GLN:HG2	1.89	0.53
1:A:107:LEU:HD12	1:A:136:TYR:O	2.08	0.53
1:C:320:ILE:HG22	1:C:330:ILE:CD1	2.38	0.53
1:D:195:ILE:HG22	1:D:256:GLU:HG3	1.89	0.53
1:D:291:ASP:OD2	1:E:207:ALA:HB1	2.08	0.53
1:E:41:PRO:CA	1:E:68:LEU:HD23	2.39	0.53
1:E:191:TYR:HB2	1:E:270:LEU:HD21	1.91	0.53
1:C:343:TRP:O	1:C:346:GLY:N	2.42	0.53
1:D:142:VAL:HG11	1:E:46:ILE:HD13	1.91	0.53
1:A:155:VAL:HG23	1:A:155:VAL:O	2.08	0.53
1:A:325:PRO:HG2	1:A:328:MET:HE2	1.91	0.53
1:A:195:ILE:HG22	1:A:256:GLU:HG3	1.91	0.52
1:D:109:THR:HG22	1:D:140:GLN:CG	2.39	0.52
1:E:188:LEU:CD2	1:E:263:ALA:HB3	2.39	0.52
1:E:134:ALA:HB1	1:E:359:TRP:HB3	1.91	0.52
1:B:109:THR:HG22	1:B:140:GLN:HG2	1.91	0.52
1:A:67:ILE:HD13	1:B:172:TYR:CD2	2.44	0.52
1:C:286:LYS:HA	1:C:293:ARG:NH1	2.07	0.52
1:E:343:TRP:O	1:E:346:GLY:N	2.42	0.52
1:E:74:ILE:HD11	1:E:79:VAL:HG22	1.92	0.52
1:D:286:LYS:HA	1:D:293:ARG:NH1	2.07	0.52
1:D:74:ILE:HD11	1:D:79:VAL:HG22	1.92	0.52
1:E:107:LEU:HD12	1:E:136:TYR:O	2.09	0.52
1:C:107:LEU:HD12	1:C:136:TYR:O	2.09	0.52
1:C:109:THR:HG22	1:C:140:GLN:CG	2.39	0.52
1:D:321:THR:OG1	1:D:330:ILE:HD12	2.09	0.52
1:D:41:PRO:CA	1:D:68:LEU:HD23	2.40	0.52
1:E:321:THR:OG1	1:E:330:ILE:HD12	2.09	0.52
1:A:343:TRP:O	1:A:346:GLY:N	2.42	0.52
1:B:78:ILE:HA	1:B:118:ASN:ND2	2.24	0.52
1:B:278:HIS:CD2	1:B:279:THR:HG23	2.44	0.52
1:C:278:HIS:CD2	1:C:279:THR:HG23	2.44	0.52
1:D:343:TRP:O	1:D:346:GLY:N	2.43	0.52
1:B:155:VAL:HG23	1:B:155:VAL:O	2.10	0.52
1:C:320:ILE:O	1:C:323:LEU:N	2.43	0.52
1:D:155:VAL:HG23	1:D:155:VAL:O	2.10	0.52
1:D:183:LEU:CD2	1:D:270:LEU:HD12	2.32	0.52
1:E:195:ILE:HG22	1:E:256:GLU:HG3	1.91	0.52
1:A:134:ALA:HB1	1:A:359:TRP:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HD11	1:B:79:VAL:HG22	1.92	0.51
1:D:134:ALA:HB1	1:D:359:TRP:HB3	1.92	0.51
1:D:188:LEU:CD2	1:D:263:ALA:HB3	2.40	0.51
1:A:11:LEU:O	1:A:106:VAL:HA	2.11	0.51
1:A:320:ILE:CG2	1:A:330:ILE:HD13	2.41	0.51
1:A:41:PRO:CA	1:A:68:LEU:HD23	2.39	0.51
1:B:188:LEU:CD2	1:B:263:ALA:HB3	2.40	0.51
1:B:320:ILE:CG2	1:B:330:ILE:HD13	2.40	0.51
1:C:155:VAL:HG23	1:C:155:VAL:O	2.09	0.51
1:C:160:ASP:HB3	1:C:186:ARG:HG3	1.93	0.51
1:C:191:TYR:HB2	1:C:270:LEU:HD21	1.91	0.51
1:A:168:ILE:HG23	1:A:172:TYR:O	2.11	0.51
1:A:188:LEU:CD2	1:A:263:ALA:HB3	2.41	0.51
1:B:160:ASP:HB3	1:B:186:ARG:HG3	1.92	0.51
1:B:343:TRP:O	1:B:346:GLY:N	2.42	0.51
1:C:56:PHE:HE2	1:C:64:LYS:HD2	1.74	0.51
1:C:168:ILE:HG23	1:C:172:TYR:O	2.11	0.51
1:C:41:PRO:CA	1:C:68:LEU:HD23	2.40	0.51
1:B:41:PRO:CA	1:B:68:LEU:HD23	2.40	0.51
1:E:320:ILE:O	1:E:323:LEU:N	2.44	0.51
1:C:320:ILE:CG2	1:C:330:ILE:HD13	2.41	0.51
1:E:155:VAL:HG23	1:E:155:VAL:O	2.10	0.51
1:B:107:LEU:HD12	1:B:136:TYR:O	2.10	0.51
1:C:11:LEU:O	1:C:106:VAL:HA	2.11	0.51
1:D:320:ILE:O	1:D:323:LEU:N	2.44	0.51
1:E:168:ILE:HG23	1:E:172:TYR:O	2.11	0.51
1:A:160:ASP:HB3	1:A:186:ARG:HG3	1.93	0.51
1:A:291:ASP:OD2	1:C:207:ALA:HB1	2.10	0.51
1:B:320:ILE:O	1:B:323:LEU:N	2.44	0.51
1:C:279:THR:O	1:C:283:ASN:HB2	2.11	0.51
1:C:74:ILE:HD11	1:C:79:VAL:HG22	1.92	0.51
1:E:109:THR:HG22	1:E:140:GLN:CG	2.40	0.51
1:A:74:ILE:CD1	1:A:79:VAL:HG22	2.41	0.51
1:A:191:TYR:HB2	1:A:270:LEU:HD21	1.91	0.50
1:E:278:HIS:CD2	1:E:279:THR:HG23	2.45	0.50
1:A:183:LEU:CD2	1:A:270:LEU:HD12	2.35	0.50
1:C:134:ALA:HB1	1:C:359:TRP:HB3	1.91	0.50
1:A:109:THR:HG22	1:A:140:GLN:CG	2.41	0.50
1:B:11:LEU:O	1:B:106:VAL:HA	2.12	0.50
1:C:188:LEU:CD2	1:C:263:ALA:HB3	2.41	0.50
1:D:168:ILE:HG23	1:D:172:TYR:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ILE:HA	1:D:118:ASN:ND2	2.23	0.50
1:B:191:TYR:HB2	1:B:270:LEU:HD21	1.92	0.50
1:D:107:LEU:HD12	1:D:136:TYR:O	2.11	0.50
1:A:320:ILE:O	1:A:323:LEU:N	2.44	0.50
1:D:116:LYS:HE3	1:D:374:HIS:NE2	2.26	0.50
1:E:320:ILE:CG2	1:E:330:ILE:HD13	2.40	0.50
1:E:78:ILE:HA	1:E:118:ASN:ND2	2.24	0.50
1:A:321:THR:HA	1:A:330:ILE:HD12	1.94	0.50
1:B:321:THR:CA	1:B:330:ILE:HD12	2.42	0.50
1:C:321:THR:CA	1:C:330:ILE:HD12	2.42	0.50
1:B:321:THR:HA	1:B:330:ILE:HD12	1.94	0.50
1:B:134:ALA:HB1	1:B:359:TRP:HB3	1.92	0.50
1:C:198:GLU:CG	1:E:116:LYS:HD2	2.42	0.50
1:D:191:TYR:OH	1:D:195:ILE:HD11	2.11	0.50
1:A:321:THR:CA	1:A:330:ILE:HD12	2.42	0.50
1:B:168:ILE:HG23	1:B:172:TYR:O	2.12	0.50
1:D:321:THR:HA	1:D:330:ILE:HD12	1.93	0.50
1:E:20:VAL:HG23	1:E:36:SER:HB3	1.94	0.50
1:A:282:PHE:O	1:A:286:LYS:HG2	2.12	0.49
1:C:321:THR:HA	1:C:330:ILE:HD12	1.94	0.49
1:D:321:THR:CA	1:D:330:ILE:HD12	2.42	0.49
1:A:247:ASP:O	1:B:328:MET:SD	2.71	0.49
1:A:279:THR:O	1:A:283:ASN:HB2	2.12	0.49
1:B:109:THR:HG22	1:B:140:GLN:CG	2.41	0.49
1:C:282:PHE:O	1:C:286:LYS:HG2	2.12	0.49
1:E:321:THR:HA	1:E:330:ILE:HD12	1.94	0.49
1:E:160:ASP:HB3	1:E:186:ARG:HG3	1.94	0.49
1:A:20:VAL:HG23	1:A:36:SER:HB3	1.94	0.49
1:A:56:PHE:HE2	1:A:64:LYS:HD2	1.77	0.49
1:B:112:PRO:HD2	1:B:164:HIS:NE2	2.27	0.49
1:C:364:GLU:HG3	1:C:372:ILE:HD13	1.93	0.49
1:D:11:LEU:O	1:D:106:VAL:HA	2.11	0.49
1:B:282:PHE:O	1:B:286:LYS:HG2	2.13	0.49
1:C:191:TYR:OH	1:C:195:ILE:HD11	2.13	0.49
1:D:364:GLU:HG3	1:D:372:ILE:HD13	1.94	0.49
1:E:11:LEU:O	1:E:106:VAL:HA	2.12	0.49
1:E:321:THR:CA	1:E:330:ILE:HD12	2.42	0.49
1:D:282:PHE:O	1:D:286:LYS:HG2	2.12	0.49
1:D:160:ASP:HB3	1:D:186:ARG:HG3	1.94	0.49
1:E:279:THR:O	1:E:283:ASN:HB2	2.12	0.49
1:B:160:ASP:CG	2:B:401:ADP:HO3'	2.16	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HG3	1:B:291:ASP:OD2	2.13	0.49
1:D:112:PRO:CD	1:D:164:HIS:CE1	2.95	0.49
1:D:20:VAL:HG23	1:D:36:SER:HB3	1.95	0.49
1:E:137:VAL:O	1:E:137:VAL:HG23	2.13	0.49
1:E:112:PRO:CD	1:E:164:HIS:CE1	2.95	0.49
1:E:286:LYS:HA	1:E:293:ARG:NH1	2.08	0.49
1:E:282:PHE:O	1:E:286:LYS:HG2	2.12	0.49
1:B:56:PHE:HE2	1:B:64:LYS:HD2	1.78	0.49
1:E:191:TYR:OH	1:E:195:ILE:HD11	2.13	0.49
1:A:78:ILE:HA	1:A:118:ASN:ND2	2.24	0.48
1:B:282:PHE:CZ	1:B:286:LYS:HD3	2.48	0.48
1:B:364:GLU:HG3	1:B:372:ILE:HD13	1.94	0.48
1:A:327:THR:HG21	1:C:244:GLU:OE2	2.12	0.48
1:E:363:GLU:HG3	1:E:364:GLU:N	2.28	0.48
1:A:104:HIS:O	1:A:133:PRO:HD2	2.14	0.48
1:A:282:PHE:CZ	1:A:286:LYS:HD3	2.48	0.48
1:B:104:HIS:O	1:B:133:PRO:HD2	2.13	0.48
1:B:279:THR:O	1:B:283:ASN:HB2	2.12	0.48
1:B:74:ILE:CD1	1:B:79:VAL:HG22	2.43	0.48
1:C:209:LYS:O	1:C:212:VAL:HB	2.13	0.48
1:C:73:PRO:HG3	1:C:88:ILE:HD12	1.96	0.48
1:D:112:PRO:HD2	1:D:164:HIS:NE2	2.28	0.48
1:A:364:GLU:HG3	1:A:372:ILE:HD13	1.94	0.48
1:D:320:ILE:CG2	1:D:330:ILE:HD13	2.42	0.48
1:E:112:PRO:HD2	1:E:164:HIS:NE2	2.28	0.48
1:E:363:GLU:HG3	1:E:364:GLU:H	1.78	0.48
1:E:74:ILE:CD1	1:E:79:VAL:HG22	2.43	0.48
1:C:282:PHE:CZ	1:C:286:LYS:HD3	2.48	0.48
1:D:112:PRO:HG3	1:D:139:ILE:CG2	2.44	0.48
1:D:43:ASN:HB3	1:D:44:PRO:HD2	1.95	0.48
1:E:116:LYS:HE3	1:E:374:HIS:NE2	2.28	0.48
1:A:172:TYR:CD2	1:C:67:ILE:HD13	2.49	0.48
1:D:282:PHE:CZ	1:D:286:LYS:HD3	2.48	0.48
1:A:209:LYS:O	1:A:212:VAL:HB	2.13	0.48
1:A:363:GLU:HG3	1:A:364:GLU:H	1.79	0.48
1:C:137:VAL:HG23	1:C:137:VAL:O	2.13	0.48
1:D:137:VAL:HG23	1:D:137:VAL:O	2.14	0.48
1:D:74:ILE:CD1	1:D:79:VAL:HG22	2.44	0.48
1:A:112:PRO:HG3	1:A:139:ILE:CG2	2.43	0.48
1:A:106:VAL:HG12	1:A:132:VAL:HG11	1.96	0.48
1:C:206:SER:O	1:C:209:LYS:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:CD2	1:C:270:LEU:HD12	2.33	0.48
1:D:106:VAL:HG12	1:D:132:VAL:HG11	1.96	0.48
1:E:73:PRO:HG3	1:E:88:ILE:HD12	1.95	0.48
1:C:152:THR:O	1:C:299:ASN:ND2	2.46	0.48
1:E:364:GLU:HG3	1:E:372:ILE:HD13	1.95	0.48
1:A:206:SER:O	1:A:209:LYS:N	2.47	0.48
1:A:152:THR:O	1:A:299:ASN:ND2	2.46	0.48
1:B:363:GLU:HG3	1:B:364:GLU:N	2.29	0.48
1:C:224:LEU:O	1:C:315:ARG:NH1	2.47	0.48
1:D:209:LYS:O	1:D:212:VAL:HB	2.14	0.48
1:D:73:PRO:HG3	1:D:88:ILE:HD12	1.96	0.48
1:E:152:THR:O	1:E:299:ASN:ND2	2.46	0.48
1:E:188:LEU:HD11	1:E:264:LEU:CG	2.44	0.48
1:E:282:PHE:CZ	1:E:286:LYS:HD3	2.48	0.48
1:B:112:PRO:HG3	1:B:139:ILE:CG2	2.43	0.48
1:B:112:PRO:CD	1:B:164:HIS:CE1	2.95	0.47
1:B:192:LEU:O	1:B:196:LEU:HB2	2.13	0.47
1:B:206:SER:O	1:B:209:LYS:N	2.47	0.47
1:C:363:GLU:HG3	1:C:364:GLU:H	1.79	0.47
1:A:137:VAL:O	1:A:137:VAL:HG23	2.13	0.47
1:B:116:LYS:HE3	1:B:374:HIS:NE2	2.29	0.47
1:B:152:THR:O	1:B:299:ASN:ND2	2.47	0.47
1:C:20:VAL:HG23	1:C:36:SER:HB3	1.96	0.47
1:D:279:THR:O	1:D:283:ASN:HB2	2.13	0.47
1:E:209:LYS:O	1:E:212:VAL:HB	2.14	0.47
1:A:363:GLU:HG3	1:A:364:GLU:N	2.29	0.47
1:C:74:ILE:CD1	1:C:79:VAL:HG22	2.45	0.47
1:D:192:LEU:O	1:D:196:LEU:HB2	2.14	0.47
1:E:43:ASN:HB3	1:E:44:PRO:HD2	1.97	0.47
1:B:192:LEU:HD13	1:B:260:CYS:HB2	1.97	0.47
1:C:112:PRO:HG3	1:C:139:ILE:CG2	2.44	0.47
1:D:188:LEU:HD11	1:D:264:LEU:CG	2.44	0.47
1:A:191:TYR:OH	1:A:195:ILE:HD11	2.15	0.47
1:B:106:VAL:HG12	1:B:132:VAL:HG11	1.97	0.47
1:B:191:TYR:OH	1:B:195:ILE:HD11	2.13	0.47
1:C:126:MET:HB3	1:C:135:MET:HE3	1.95	0.47
1:D:152:THR:O	1:D:299:ASN:ND2	2.47	0.47
1:E:112:PRO:HG3	1:E:139:ILE:CG2	2.45	0.47
1:A:112:PRO:HD2	1:A:164:HIS:NE2	2.28	0.47
1:B:118:ASN:O	1:B:122:MET:CB	2.63	0.47
1:B:209:LYS:O	1:B:212:VAL:HB	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:HG3	1:B:364:GLU:H	1.79	0.47
1:C:43:ASN:HB3	1:C:44:PRO:HD2	1.96	0.47
1:D:224:LEU:O	1:D:315:ARG:NH1	2.48	0.47
1:D:363:GLU:HG3	1:D:364:GLU:N	2.29	0.47
1:E:106:VAL:HG12	1:E:132:VAL:HG11	1.97	0.47
1:E:192:LEU:O	1:E:196:LEU:HB2	2.14	0.47
1:E:104:HIS:O	1:E:133:PRO:HD2	2.14	0.47
1:A:116:LYS:HE3	1:A:374:HIS:NE2	2.30	0.47
1:C:192:LEU:O	1:C:196:LEU:HB2	2.15	0.47
1:C:363:GLU:HG3	1:C:364:GLU:N	2.29	0.47
1:E:224:LEU:O	1:E:315:ARG:NH1	2.48	0.47
1:A:220:CYS:HB3	1:A:261:PRO:CG	2.45	0.47
1:B:219:LEU:CD1	1:B:243:TYR:HB2	2.42	0.47
1:B:220:CYS:HB3	1:B:261:PRO:CG	2.44	0.47
1:B:188:LEU:HD11	1:B:264:LEU:CG	2.44	0.47
1:B:20:VAL:HG23	1:B:36:SER:HB3	1.96	0.47
1:C:112:PRO:HD2	1:C:164:HIS:NE2	2.29	0.47
1:E:220:CYS:HB3	1:E:261:PRO:CG	2.45	0.47
1:B:11:LEU:HD11	1:B:97:LEU:HD13	1.96	0.47
1:D:206:SER:O	1:D:209:LYS:N	2.47	0.47
1:E:206:SER:O	1:E:209:LYS:N	2.47	0.47
1:E:183:LEU:CD2	1:E:270:LEU:HD12	2.34	0.47
1:A:118:ASN:O	1:A:122:MET:CB	2.63	0.46
1:A:192:LEU:O	1:A:196:LEU:HB2	2.15	0.46
1:A:333:VAL:O	1:A:333:VAL:HG13	2.15	0.46
1:C:106:VAL:HG12	1:C:132:VAL:HG11	1.97	0.46
1:C:201:TYR:CZ	1:C:251:ILE:HG23	2.49	0.46
1:D:154:ILE:O	1:D:301:VAL:HG22	2.15	0.46
1:E:333:VAL:HG13	1:E:333:VAL:O	2.15	0.46
1:B:333:VAL:O	1:B:333:VAL:HG13	2.16	0.46
1:C:118:ASN:O	1:C:122:MET:CB	2.63	0.46
1:C:226:PHE:CD1	1:C:262:GLU:OE1	2.69	0.46
1:C:188:LEU:HD11	1:C:264:LEU:CG	2.45	0.46
1:D:138:ALA:HB1	1:D:143:LEU:HD11	1.96	0.46
1:D:220:CYS:HB3	1:D:261:PRO:CG	2.45	0.46
1:D:104:HIS:O	1:D:133:PRO:HD2	2.14	0.46
1:D:279:THR:O	1:D:283:ASN:CB	2.64	0.46
1:A:43:ASN:HB3	1:A:44:PRO:HD2	1.97	0.46
1:A:73:PRO:HG3	1:A:88:ILE:HD12	1.98	0.46
1:B:137:VAL:HG23	1:B:137:VAL:O	2.14	0.46
1:B:188:LEU:HD11	1:B:264:LEU:HG	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASN:HB3	1:B:44:PRO:HD2	1.97	0.46
1:B:224:LEU:O	1:B:315:ARG:NH1	2.49	0.46
1:C:279:THR:O	1:C:283:ASN:CB	2.64	0.46
1:C:67:ILE:HG22	1:C:67:ILE:O	2.16	0.46
1:A:220:CYS:HB3	1:A:261:PRO:HG2	1.98	0.46
1:A:188:LEU:HD11	1:A:264:LEU:CG	2.45	0.46
1:A:224:LEU:O	1:A:315:ARG:NH1	2.49	0.46
1:A:67:ILE:O	1:A:67:ILE:HG22	2.16	0.46
1:B:226:PHE:CD1	1:B:262:GLU:OE1	2.69	0.46
1:C:104:HIS:O	1:C:133:PRO:HD2	2.15	0.46
1:C:220:CYS:HB3	1:C:261:PRO:CG	2.45	0.46
1:E:226:PHE:CD1	1:E:262:GLU:OE1	2.69	0.46
1:A:201:TYR:CZ	1:A:251:ILE:HG23	2.50	0.46
1:B:138:ALA:HB1	1:B:143:LEU:HD11	1.96	0.46
1:C:138:ALA:HB1	1:C:143:LEU:HD11	1.96	0.46
1:A:112:PRO:CD	1:A:164:HIS:CE1	2.95	0.46
1:A:226:PHE:CD1	1:A:262:GLU:OE1	2.69	0.46
1:B:145:LEU:HB2	1:B:155:VAL:HG11	1.98	0.46
1:B:220:CYS:HB3	1:B:261:PRO:HG2	1.98	0.46
1:C:223:ALA:O	1:C:315:ARG:HD2	2.16	0.46
1:D:192:LEU:HD13	1:D:260:CYS:HB2	1.96	0.46
1:B:73:PRO:HG3	1:B:88:ILE:HD12	1.97	0.46
1:E:56:PHE:HE2	1:E:64:LYS:HD2	1.76	0.46
1:A:223:ALA:O	1:A:315:ARG:HD2	2.16	0.46
1:E:279:THR:O	1:E:283:ASN:CB	2.64	0.46
1:E:223:ALA:O	1:E:315:ARG:HD2	2.16	0.46
1:A:192:LEU:HD13	1:A:260:CYS:HB2	1.98	0.45
1:A:279:THR:O	1:A:283:ASN:CB	2.64	0.45
1:B:363:GLU:O	1:B:366:ASP:N	2.50	0.45
1:C:116:LYS:HE3	1:C:374:HIS:NE2	2.31	0.45
1:C:192:LEU:HD13	1:C:260:CYS:HB2	1.99	0.45
1:D:150:ARG:NH1	1:D:299:ASN:OD1	2.49	0.45
1:D:291:ASP:OD2	1:E:65:ARG:HG3	2.17	0.45
1:A:126:MET:HB3	1:A:135:MET:HE3	1.97	0.45
1:B:67:ILE:O	1:B:67:ILE:HG22	2.17	0.45
1:C:220:CYS:HB3	1:C:261:PRO:HG2	1.98	0.45
1:D:56:PHE:HE2	1:D:64:LYS:HD2	1.76	0.45
1:E:305:GLY:O	1:E:308:MET:HG2	2.15	0.45
1:E:67:ILE:O	1:E:67:ILE:HG22	2.16	0.45
1:A:154:ILE:O	1:A:301:VAL:HG22	2.16	0.45
1:B:223:ALA:O	1:B:315:ARG:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:THR:O	1:B:283:ASN:CB	2.64	0.45
1:B:150:ARG:NH1	1:B:299:ASN:OD1	2.50	0.45
4:C:403:9UE:BR	1:E:76:HIS:CD2	3.24	0.45
1:D:11:LEU:HD11	1:D:97:LEU:HD13	1.97	0.45
1:D:118:ASN:O	1:D:122:MET:CB	2.64	0.45
1:D:226:PHE:CD1	1:D:262:GLU:OE1	2.69	0.45
1:D:223:ALA:O	1:D:315:ARG:HD2	2.17	0.45
1:D:363:GLU:HG3	1:D:364:GLU:H	1.80	0.45
1:D:363:GLU:O	1:D:366:ASP:N	2.49	0.45
1:E:220:CYS:HB3	1:E:261:PRO:HG2	1.98	0.45
1:E:150:ARG:NH1	1:E:299:ASN:OD1	2.50	0.45
1:A:305:GLY:O	1:A:308:MET:HG2	2.16	0.45
1:C:333:VAL:HG13	1:C:333:VAL:O	2.15	0.45
1:C:363:GLU:O	1:C:366:ASP:N	2.50	0.45
1:E:192:LEU:HD13	1:E:260:CYS:HB2	1.97	0.45
1:A:138:ALA:HB1	1:A:143:LEU:HD11	1.97	0.45
1:B:305:GLY:O	1:B:308:MET:HG2	2.16	0.45
1:C:11:LEU:HD11	1:C:97:LEU:HD13	1.98	0.45
1:D:188:LEU:HD11	1:D:264:LEU:HG	1.99	0.45
1:E:138:ALA:HB1	1:E:143:LEU:HD11	1.98	0.45
1:A:169:TYR:HD2	1:C:67:ILE:CD1	2.25	0.45
1:A:8:VAL:O	1:A:8:VAL:HG12	2.17	0.45
1:D:106:VAL:HG13	1:D:135:MET:HE2	1.98	0.45
1:E:188:LEU:HD11	1:E:264:LEU:HG	1.97	0.45
1:A:150:ARG:NH1	1:A:299:ASN:OD1	2.50	0.45
1:B:262:GLU:HG2	1:B:262:GLU:O	2.17	0.45
1:C:154:ILE:O	1:C:301:VAL:HG22	2.16	0.45
1:A:11:LEU:HD11	1:A:97:LEU:HD13	1.98	0.45
1:C:188:LEU:HD11	1:C:264:LEU:HG	1.99	0.45
1:D:305:GLY:O	1:D:308:MET:HG2	2.16	0.45
1:D:333:VAL:O	1:D:333:VAL:HG13	2.16	0.45
1:E:8:VAL:HG12	1:E:8:VAL:O	2.17	0.45
1:A:145:LEU:HB2	1:A:155:VAL:HG11	1.99	0.45
1:A:363:GLU:O	1:A:366:ASP:N	2.49	0.45
1:C:112:PRO:CD	1:C:164:HIS:CE1	2.96	0.45
1:D:201:TYR:CZ	1:D:251:ILE:HG23	2.52	0.45
1:D:262:GLU:O	1:D:262:GLU:HG2	2.17	0.45
1:E:363:GLU:O	1:E:366:ASP:N	2.50	0.45
1:C:150:ARG:NH1	1:C:299:ASN:OD1	2.50	0.44
1:E:118:ASN:O	1:E:122:MET:CB	2.65	0.44
1:D:8:VAL:O	1:D:8:VAL:HG12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ILE:O	1:E:301:VAL:HG22	2.17	0.44
1:A:188:LEU:HD11	1:A:264:LEU:HG	1.98	0.44
1:C:8:VAL:HG12	1:C:8:VAL:O	2.17	0.44
1:D:220:CYS:HB3	1:D:261:PRO:HG2	1.98	0.44
1:A:262:GLU:O	1:A:262:GLU:HG2	2.17	0.44
1:A:293:ARG:HB3	1:A:297:TYR:HE2	1.83	0.44
1:B:112:PRO:HG3	1:B:139:ILE:HG23	1.99	0.44
1:B:154:ILE:O	1:B:301:VAL:HG22	2.18	0.44
1:B:293:ARG:HB3	1:B:297:TYR:CE2	2.53	0.44
1:D:67:ILE:O	1:D:67:ILE:HG22	2.17	0.44
1:B:286:LYS:HD2	1:B:293:ARG:NH1	2.33	0.44
1:C:262:GLU:O	1:C:262:GLU:HG2	2.17	0.44
1:C:305:GLY:O	1:C:308:MET:HG2	2.17	0.44
1:E:286:LYS:HD2	1:E:293:ARG:NH1	2.33	0.44
1:B:8:VAL:HG12	1:B:8:VAL:O	2.17	0.44
1:E:145:LEU:HB2	1:E:155:VAL:HG11	2.00	0.44
1:C:145:LEU:HB2	1:C:155:VAL:HG11	2.00	0.44
1:D:145:LEU:HB2	1:D:155:VAL:HG11	2.00	0.44
1:A:64:LYS:CG	1:A:64:LYS:O	2.66	0.44
1:B:154:ILE:CD1	1:B:285:ILE:HG13	2.44	0.44
1:C:293:ARG:HB3	1:C:297:TYR:CE2	2.53	0.44
1:E:201:TYR:CZ	1:E:251:ILE:HG23	2.51	0.44
1:A:74:ILE:O	1:A:186:ARG:NH1	2.51	0.43
1:A:67:ILE:CD1	1:B:169:TYR:HD2	2.28	0.43
1:D:193:MET:CE	1:D:209:LYS:HA	2.48	0.43
1:D:321:THR:HA	1:D:330:ILE:CD1	2.48	0.43
1:E:293:ARG:HB3	1:E:297:TYR:CE2	2.53	0.43
1:A:112:PRO:HG3	1:A:139:ILE:HG23	2.00	0.43
1:A:193:MET:CE	1:A:209:LYS:HA	2.48	0.43
1:A:293:ARG:HB3	1:A:297:TYR:CE2	2.53	0.43
1:D:162:VAL:HG12	1:D:163:SER:N	2.33	0.43
1:D:183:LEU:HD11	1:D:267:PRO:CB	2.32	0.43
1:E:106:VAL:HG13	1:E:135:MET:HE2	2.00	0.43
1:E:193:MET:CE	1:E:209:LYS:HA	2.48	0.43
1:A:219:LEU:CD1	1:A:243:TYR:HB2	2.43	0.43
1:C:74:ILE:O	1:C:186:ARG:NH1	2.51	0.43
1:A:321:THR:HA	1:A:330:ILE:CD1	2.49	0.43
1:C:64:LYS:CG	1:C:64:LYS:O	2.67	0.43
1:E:11:LEU:HD11	1:E:97:LEU:HD13	1.99	0.43
1:E:293:ARG:HB3	1:E:297:TYR:HE2	1.83	0.43
1:C:193:MET:CE	1:C:209:LYS:HA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:HD2	1:A:293:ARG:NH1	2.33	0.43
1:A:142:VAL:HG11	1:C:46:ILE:CD1	2.46	0.43
1:B:321:THR:HA	1:B:330:ILE:CD1	2.49	0.43
1:D:293:ARG:HB3	1:D:297:TYR:CE2	2.54	0.43
1:E:301:VAL:CG2	1:E:301:VAL:O	2.66	0.43
1:D:286:LYS:HD2	1:D:293:ARG:NH1	2.33	0.43
1:E:162:VAL:HG12	1:E:163:SER:N	2.34	0.43
1:E:321:THR:HA	1:E:330:ILE:CD1	2.48	0.43
1:E:64:LYS:O	1:E:64:LYS:CG	2.66	0.43
1:A:317:THR:HG22	1:A:332:VAL:HG13	2.01	0.43
1:A:34:PHE:CZ	1:A:92:THR:HG22	2.54	0.43
1:D:74:ILE:O	1:D:186:ARG:NH1	2.52	0.43
1:E:262:GLU:O	1:E:262:GLU:HG2	2.17	0.43
1:A:192:LEU:HD23	1:A:212:VAL:HG13	2.01	0.43
1:B:192:LEU:HD23	1:B:212:VAL:HG13	2.01	0.43
1:D:112:PRO:HG3	1:D:139:ILE:HG23	2.00	0.43
1:E:363:GLU:CG	1:E:364:GLU:H	2.32	0.43
1:A:155:VAL:HA	1:A:301:VAL:CG2	2.49	0.42
1:C:293:ARG:HB3	1:C:297:TYR:HE2	1.83	0.42
1:C:321:THR:HA	1:C:330:ILE:CD1	2.49	0.42
1:E:74:ILE:O	1:E:186:ARG:NH1	2.52	0.42
1:B:162:VAL:HG12	1:B:163:SER:N	2.33	0.42
1:B:293:ARG:HB3	1:B:297:TYR:HE2	1.83	0.42
1:D:155:VAL:HA	1:D:301:VAL:CG2	2.49	0.42
1:D:301:VAL:CG2	1:D:301:VAL:O	2.67	0.42
1:B:64:LYS:O	1:B:64:LYS:CG	2.67	0.42
1:C:112:PRO:HG3	1:C:139:ILE:HG23	2.00	0.42
1:A:162:VAL:HG12	1:A:163:SER:N	2.34	0.42
1:C:155:VAL:HA	1:C:301:VAL:CG2	2.50	0.42
1:C:93:PHE:HD1	1:C:97:LEU:HD12	1.84	0.42
1:B:126:MET:HB3	1:B:135:MET:HE3	2.01	0.42
1:C:286:LYS:HD2	1:C:293:ARG:NH1	2.35	0.42
1:D:293:ARG:HB3	1:D:297:TYR:HE2	1.85	0.42
1:E:156:LEU:HA	1:E:164:HIS:O	2.20	0.42
1:E:317:THR:HG22	1:E:332:VAL:HG13	2.02	0.42
1:A:301:VAL:CG2	1:A:301:VAL:O	2.66	0.42
1:B:193:MET:CE	1:B:209:LYS:HA	2.49	0.42
1:B:201:TYR:CZ	1:B:251:ILE:HG23	2.54	0.42
1:C:192:LEU:HD23	1:C:212:VAL:HG13	2.01	0.42
1:D:193:MET:CE	1:D:209:LYS:HB2	2.50	0.42
1:E:219:LEU:CD1	1:E:243:TYR:HB2	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HD1	1:A:97:LEU:HD12	1.85	0.42
1:B:317:THR:HG22	1:B:332:VAL:HG13	2.02	0.42
1:C:139:ILE:O	1:C:142:VAL:HG22	2.20	0.42
1:C:162:VAL:HG12	1:C:163:SER:N	2.34	0.42
1:D:317:THR:HG22	1:D:332:VAL:HG13	2.02	0.42
1:D:328:MET:SD	1:E:247:ASP:O	2.77	0.42
1:D:85:MET:O	1:D:88:ILE:N	2.53	0.42
1:D:93:PHE:HD1	1:D:97:LEU:HD12	1.84	0.42
1:B:363:GLU:CG	1:B:364:GLU:H	2.33	0.42
1:B:74:ILE:HD11	1:B:85:MET:HE3	2.02	0.42
1:C:317:THR:HG22	1:C:332:VAL:HG13	2.02	0.42
1:E:85:MET:O	1:E:88:ILE:N	2.53	0.42
1:A:332:VAL:CG2	1:A:332:VAL:O	2.68	0.41
1:C:301:VAL:CG2	1:C:301:VAL:O	2.66	0.41
1:C:85:MET:O	1:C:88:ILE:N	2.52	0.41
1:D:156:LEU:HA	1:D:164:HIS:O	2.20	0.41
1:E:197:HIS:HA	1:E:201:TYR:O	2.20	0.41
1:A:183:LEU:HD21	1:A:272:LYS:HD2	2.02	0.41
1:B:18:GLY:O	1:B:19:ASN:OD1	2.38	0.41
1:C:109:THR:CG2	1:C:140:GLN:CG	2.97	0.41
1:C:196:LEU:HD12	1:C:196:LEU:HA	1.94	0.41
1:E:93:PHE:HD1	1:E:97:LEU:HD12	1.84	0.41
1:B:85:MET:O	1:B:88:ILE:N	2.53	0.41
1:E:183:LEU:HD21	1:E:272:LYS:HD2	2.03	0.41
1:A:156:LEU:HA	1:A:164:HIS:O	2.21	0.41
1:A:363:GLU:CG	1:A:364:GLU:H	2.33	0.41
1:B:299:ASN:O	1:B:300:ILE:C	2.59	0.41
1:B:74:ILE:O	1:B:186:ARG:NH1	2.54	0.41
1:D:363:GLU:CG	1:D:364:GLU:H	2.33	0.41
1:A:156:LEU:HD12	1:A:156:LEU:O	2.21	0.41
1:B:156:LEU:HA	1:B:164:HIS:O	2.20	0.41
1:C:18:GLY:O	1:C:19:ASN:OD1	2.38	0.41
1:C:197:HIS:HA	1:C:201:TYR:O	2.21	0.41
1:D:169:TYR:HD2	1:E:67:ILE:CD1	2.27	0.41
1:E:193:MET:CE	1:E:209:LYS:HB2	2.50	0.41
1:B:301:VAL:O	1:B:301:VAL:CG2	2.68	0.41
1:C:152:THR:CG2	1:C:295:ASP:HB3	2.50	0.41
1:C:317:THR:CG2	1:C:332:VAL:HG22	2.51	0.41
1:D:18:GLY:O	1:D:19:ASN:OD1	2.38	0.41
1:D:197:HIS:HA	1:D:201:TYR:O	2.21	0.41
1:E:18:GLY:O	1:E:19:ASN:OD1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HA	1:C:164:HIS:O	2.21	0.41
1:C:363:GLU:CG	1:C:364:GLU:H	2.33	0.41
1:E:112:PRO:HG3	1:E:139:ILE:HG23	2.01	0.41
1:E:154:ILE:CD1	1:E:285:ILE:HG13	2.44	0.41
1:A:193:MET:CE	1:A:209:LYS:HB2	2.50	0.41
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.94	0.41
1:A:74:ILE:HD11	1:A:85:MET:HE3	2.00	0.41
1:A:85:MET:O	1:A:88:ILE:N	2.53	0.41
1:B:138:ALA:HB1	1:B:143:LEU:CD1	2.50	0.41
1:B:183:LEU:HD21	1:B:272:LYS:HD2	2.03	0.41
1:B:93:PHE:HD1	1:B:97:LEU:HD12	1.85	0.41
1:C:296:LEU:HA	1:C:296:LEU:HD23	1.89	0.41
1:D:219:LEU:CD1	1:D:243:TYR:HB2	2.43	0.41
1:D:89:TRP:O	1:D:92:THR:N	2.54	0.41
1:E:89:TRP:O	1:E:92:THR:N	2.54	0.41
1:B:332:VAL:CG2	1:B:332:VAL:O	2.69	0.41
1:C:138:ALA:HB1	1:C:143:LEU:CD1	2.51	0.41
1:E:155:VAL:HA	1:E:301:VAL:CG2	2.50	0.41
1:A:112:PRO:CG	1:A:139:ILE:HG23	2.51	0.41
1:B:106:VAL:HG13	1:B:135:MET:HE2	2.02	0.41
1:B:317:THR:CG2	1:B:332:VAL:HG22	2.51	0.41
1:D:363:GLU:CG	1:D:364:GLU:N	2.84	0.41
1:D:64:LYS:O	1:D:64:LYS:CG	2.67	0.41
1:E:173:ALA:O	1:E:175:PRO:HD3	2.21	0.41
1:E:285:ILE:O	1:E:288:CYS:N	2.44	0.41
1:B:112:PRO:CG	1:B:139:ILE:HG23	2.51	0.41
1:B:155:VAL:HA	1:B:301:VAL:CG2	2.50	0.41
1:E:363:GLU:CG	1:E:364:GLU:N	2.83	0.41
1:E:34:PHE:CZ	1:E:92:THR:HG22	2.55	0.41
1:A:301:VAL:HG12	1:A:333:VAL:HG11	2.03	0.40
1:A:89:TRP:O	1:A:92:THR:N	2.54	0.40
1:B:193:MET:CE	1:B:209:LYS:HB2	2.51	0.40
1:B:363:GLU:CG	1:B:364:GLU:N	2.84	0.40
1:D:138:ALA:HB1	1:D:143:LEU:CD1	2.51	0.40
1:D:212:VAL:O	1:D:215:ILE:N	2.55	0.40
1:A:18:GLY:O	1:A:19:ASN:OD1	2.38	0.40
1:A:197:HIS:HA	1:A:201:TYR:O	2.20	0.40
1:B:34:PHE:CZ	1:B:92:THR:HG22	2.56	0.40
1:C:112:PRO:CG	1:C:139:ILE:HG23	2.52	0.40
1:E:212:VAL:O	1:E:215:ILE:N	2.54	0.40
1:A:173:ALA:O	1:A:175:PRO:HD3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:CD1	1:A:285:ILE:HG13	2.43	0.40
1:A:299:ASN:O	1:A:300:ILE:C	2.59	0.40
1:B:212:VAL:O	1:B:215:ILE:N	2.54	0.40
1:B:89:TRP:O	1:B:92:THR:N	2.55	0.40
1:C:363:GLU:CG	1:C:364:GLU:N	2.84	0.40
1:D:37:ILE:HG21	1:D:70:LEU:HD22	2.03	0.40
1:B:197:HIS:HA	1:B:201:TYR:O	2.20	0.40
1:B:306:THR:HG22	1:B:306:THR:O	2.21	0.40
1:C:219:LEU:CD1	1:C:243:TYR:HB2	2.43	0.40
1:C:89:TRP:O	1:C:92:THR:N	2.55	0.40
1:D:112:PRO:CG	1:D:139:ILE:HG23	2.51	0.40
1:D:192:LEU:HD23	1:D:212:VAL:HG13	2.02	0.40
1:E:195:ILE:HG21	1:E:256:GLU:HG3	2.03	0.40
1:A:139:ILE:O	1:A:142:VAL:HG22	2.21	0.40
1:B:37:ILE:HG21	1:B:70:LEU:HD22	2.04	0.40
1:C:34:PHE:CZ	1:C:92:THR:HG22	2.57	0.40
1:D:34:PHE:CZ	1:D:92:THR:HG22	2.56	0.40
1:E:138:ALA:HB1	1:E:143:LEU:CD1	2.51	0.40
1:E:139:ILE:O	1:E:142:VAL:HG22	2.21	0.40
1:E:192:LEU:HD23	1:E:212:VAL:HG13	2.02	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	368/378 (97%)	355 (96%)	13 (4%)	0	100	100
1	B	368/378 (97%)	355 (96%)	13 (4%)	0	100	100
1	C	368/378 (97%)	355 (96%)	13 (4%)	0	100	100
1	D	368/378 (97%)	355 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	368/378 (97%)	355 (96%)	13 (4%)	0	100	100
All	All	1840/1890 (97%)	1775 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	317/322 (98%)	317 (100%)	0	100	100
1	B	317/322 (98%)	317 (100%)	0	100	100
1	C	317/322 (98%)	317 (100%)	0	100	100
1	D	317/322 (98%)	317 (100%)	0	100	100
1	E	317/322 (98%)	317 (100%)	0	100	100
All	All	1585/1610 (98%)	1585 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	104	HIS
1	A	118	ASN
1	A	164	HIS
1	A	278	HIS
1	B	9	GLN
1	B	104	HIS
1	B	118	ASN
1	B	164	HIS
1	B	249	ASN
1	B	278	HIS
1	C	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	104	HIS
1	C	118	ASN
1	C	164	HIS
1	C	249	ASN
1	C	278	HIS
1	D	9	GLN
1	D	104	HIS
1	D	118	ASN
1	D	164	HIS
1	D	249	ASN
1	D	278	HIS
1	E	9	GLN
1	E	104	HIS
1	E	118	ASN
1	E	164	HIS
1	E	278	HIS

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](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	401	3	25,29,29	1.04	1 (4%)	24,45,45	1.45	1 (4%)
4	9UE	A	403	-	48,50,50	0.58	1 (2%)	61,71,71	1.25	6 (9%)
2	ADP	B	401	3	25,29,29	1.04	2 (8%)	24,45,45	1.44	1 (4%)
2	ADP	C	401	3	25,29,29	1.04	2 (8%)	24,45,45	1.50	1 (4%)
4	9UE	C	403	-	48,50,50	0.57	1 (2%)	61,71,71	1.25	6 (9%)
2	ADP	D	401	3	25,29,29	1.07	1 (4%)	24,45,45	1.37	1 (4%)
2	ADP	E	401	3	25,29,29	1.01	2 (8%)	24,45,45	1.58	2 (8%)
4	9UE	E	403	-	48,50,50	0.57	1 (2%)	61,71,71	1.25	6 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	401	3	-	0/12/32/32	0/3/3/3
4	9UE	A	403	-	-	0/54/56/56	0/3/4/4
2	ADP	B	401	3	-	0/12/32/32	0/3/3/3
2	ADP	C	401	3	-	0/12/32/32	0/3/3/3
4	9UE	C	403	-	-	0/54/56/56	0/3/4/4
2	ADP	D	401	3	-	0/12/32/32	0/3/3/3
2	ADP	E	401	3	-	0/12/32/32	0/3/3/3
4	9UE	E	403	-	-	0/54/56/56	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	9UE	BR-C28	-2.11	1.87	1.90
4	C	403	9UE	BR-C28	-2.08	1.87	1.90
4	E	403	9UE	BR-C28	-2.08	1.87	1.90
2	E	401	ADP	C2-N3	2.02	1.35	1.32
2	C	401	ADP	C2-N3	2.09	1.35	1.32
2	B	401	ADP	C2-N3	2.11	1.35	1.32
2	E	401	ADP	C5-C4	3.20	1.47	1.40
2	A	401	ADP	C5-C4	3.33	1.48	1.40
2	B	401	ADP	C5-C4	3.36	1.48	1.40
2	C	401	ADP	C5-C4	3.49	1.48	1.40
2	D	401	ADP	C5-C4	3.52	1.48	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	ADP	N3-C2-N1	-5.26	124.28	128.86
2	C	401	ADP	N3-C2-N1	-4.93	124.57	128.86
2	A	401	ADP	N3-C2-N1	-4.90	124.59	128.86
2	B	401	ADP	N3-C2-N1	-4.62	124.83	128.86
4	C	403	9UE	C6-N-C7	-4.24	116.68	123.16
4	E	403	9UE	C6-N-C7	-4.24	116.68	123.16
4	A	403	9UE	C6-N-C7	-4.23	116.69	123.16
2	D	401	ADP	N3-C2-N1	-3.80	125.55	128.86
4	E	403	9UE	O4-C11-C12	-2.77	115.96	121.38
4	A	403	9UE	O4-C11-C12	-2.76	115.97	121.38
4	C	403	9UE	O4-C11-C12	-2.76	115.98	121.38
2	E	401	ADP	C4-C5-N7	-2.34	107.15	109.41
4	E	403	9UE	C20-C21-C28	2.05	128.40	123.95
4	A	403	9UE	C20-C21-C28	2.05	128.41	123.95
4	C	403	9UE	C20-C21-C28	2.07	128.45	123.95
4	C	403	9UE	C10-N2-C11	2.27	126.23	121.27
4	A	403	9UE	C10-N2-C11	2.27	126.24	121.27
4	E	403	9UE	C10-N2-C11	2.29	126.28	121.27
4	E	403	9UE	C5-C6-C29	3.14	119.00	111.73
4	A	403	9UE	C5-C6-C29	3.15	119.02	111.73
4	C	403	9UE	C5-C6-C29	3.17	119.08	111.73
4	A	403	9UE	C12-C11-N2	3.44	120.16	116.40
4	E	403	9UE	C12-C11-N2	3.47	120.19	116.40
4	C	403	9UE	C12-C11-N2	3.48	120.21	116.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	1	0
2	B	401	ADP	2	0
2	C	401	ADP	1	0
4	C	403	9UE	4	0
2	D	401	ADP	1	0
2	E	401	ADP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.