



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:23 AM EST

PDB ID : 3J8I
EMDB ID : EMD-6179
Title : Near-Atomic Resolution for One State of F-Actin
Authors : Galkin, V.E.
Deposited on : 2014-11-06
Resolution : 4.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

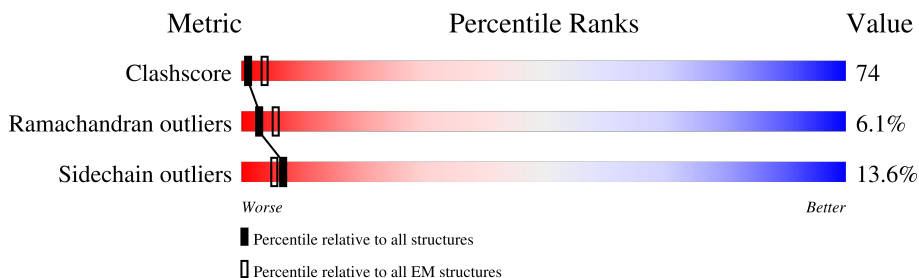
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	377	<div> <div>20%</div> <div>22%</div> <div>62%</div> <div>14%</div> <div>..</div> </div>
1	E	377	<div> <div>20%</div> <div>23%</div> <div>62%</div> <div>14%</div> <div>..</div> </div>
1	F	377	<div> <div>19%</div> <div>21%</div> <div>64%</div> <div>14%</div> <div>..</div> </div>
1	G	377	<div> <div>18%</div> <div>23%</div> <div>62%</div> <div>14%</div> <div>..</div> </div>
1	H	377	<div> <div>18%</div> <div>21%</div> <div>64%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition [i](#)

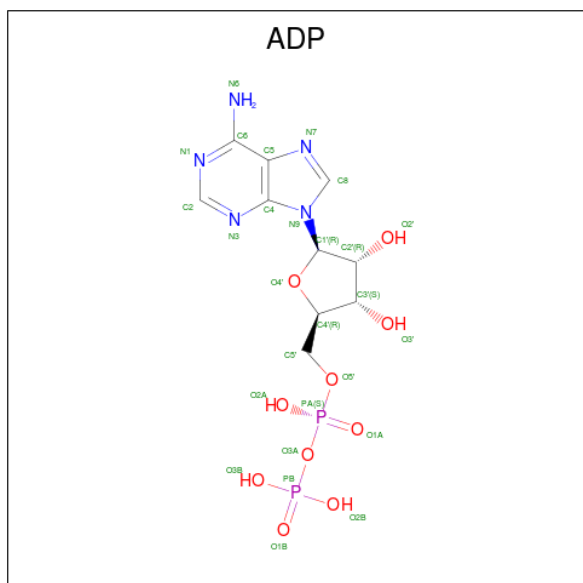
There are 3 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	375	Total	C	N	O	S	0	0
			2932	1854	493	564	21		
1	E	375	Total	C	N	O	S	0	0
			2932	1854	493	564	21		
1	F	375	Total	C	N	O	S	0	0
			2932	1854	493	564	21		
1	G	375	Total	C	N	O	S	0	0
			2932	1854	493	564	21		
1	H	375	Total	C	N	O	S	0	0
			2932	1854	493	564	21		

- 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	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

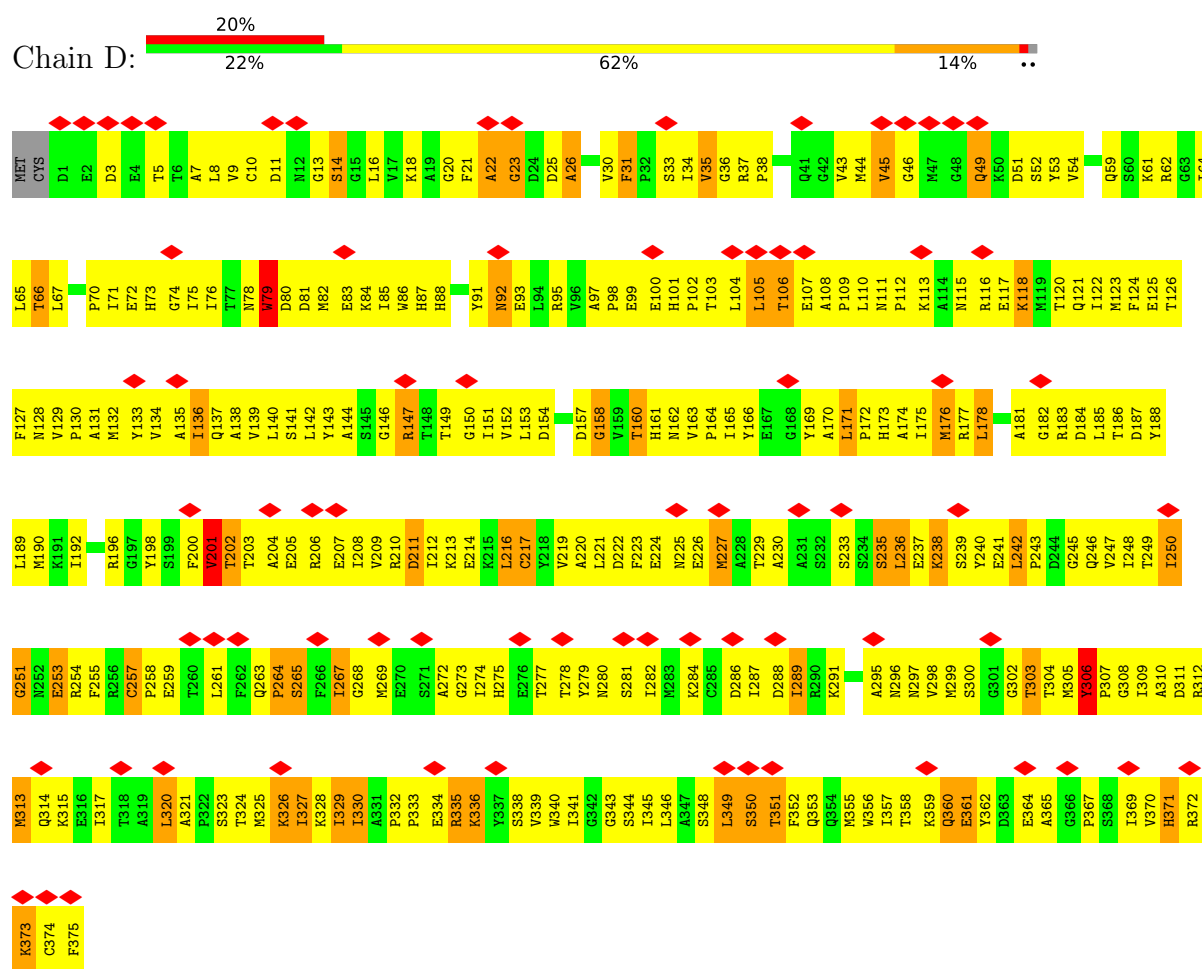
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	G	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	

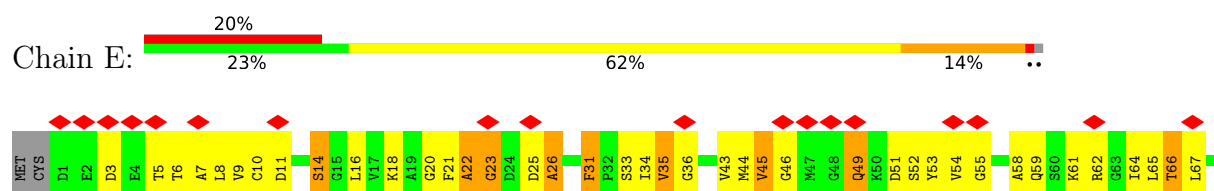
3 Residue-property plots [i](#)

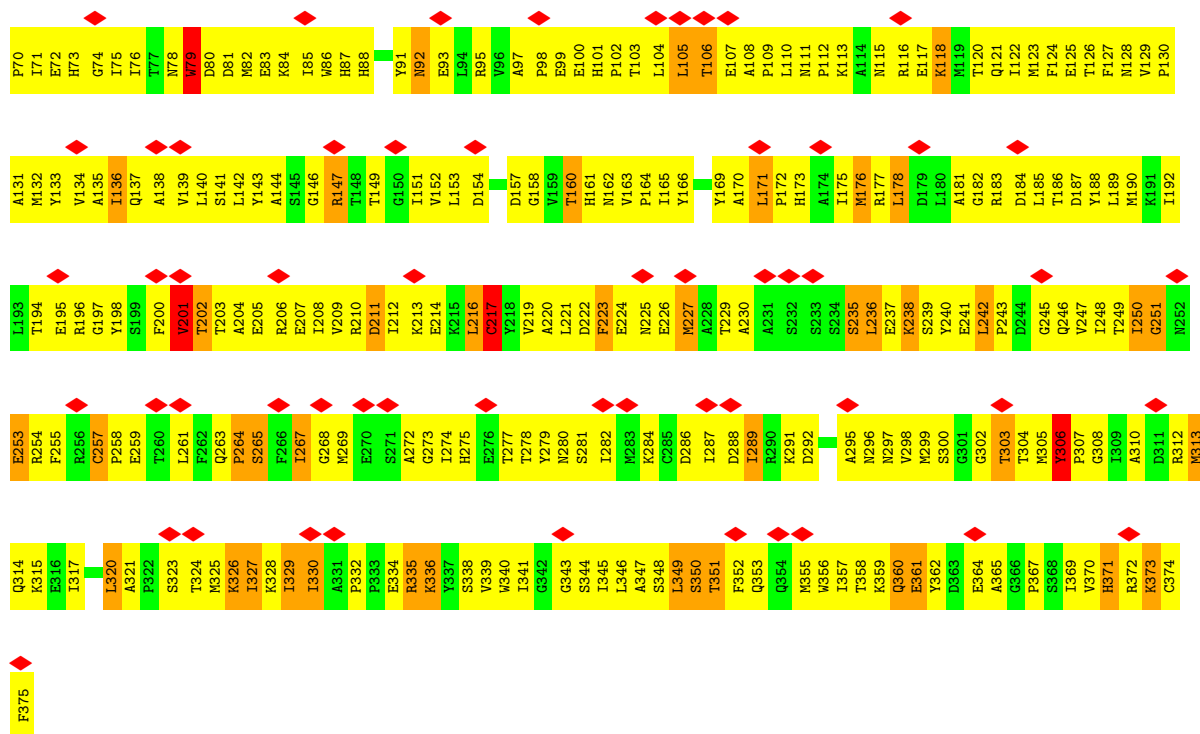
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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, alpha skeletal muscle

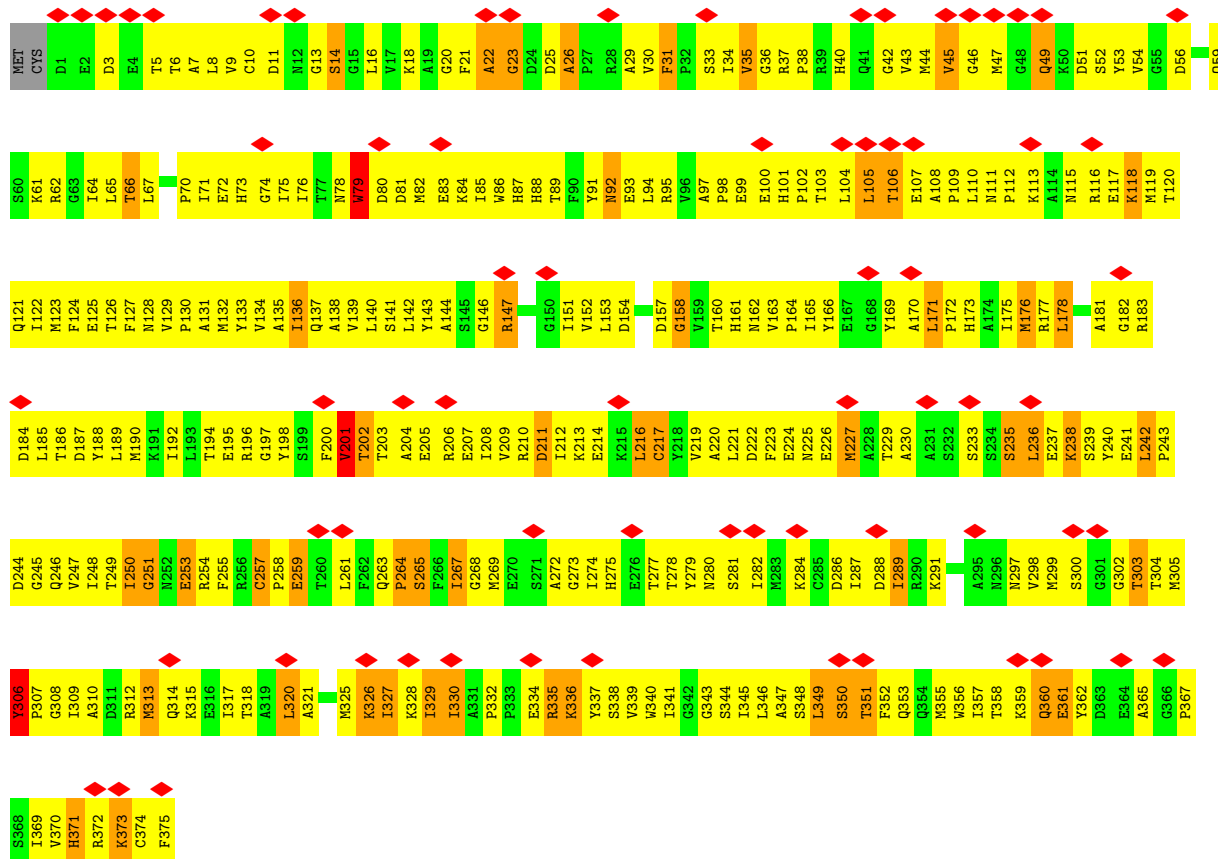


• Molecule 1: Actin, alpha skeletal muscle

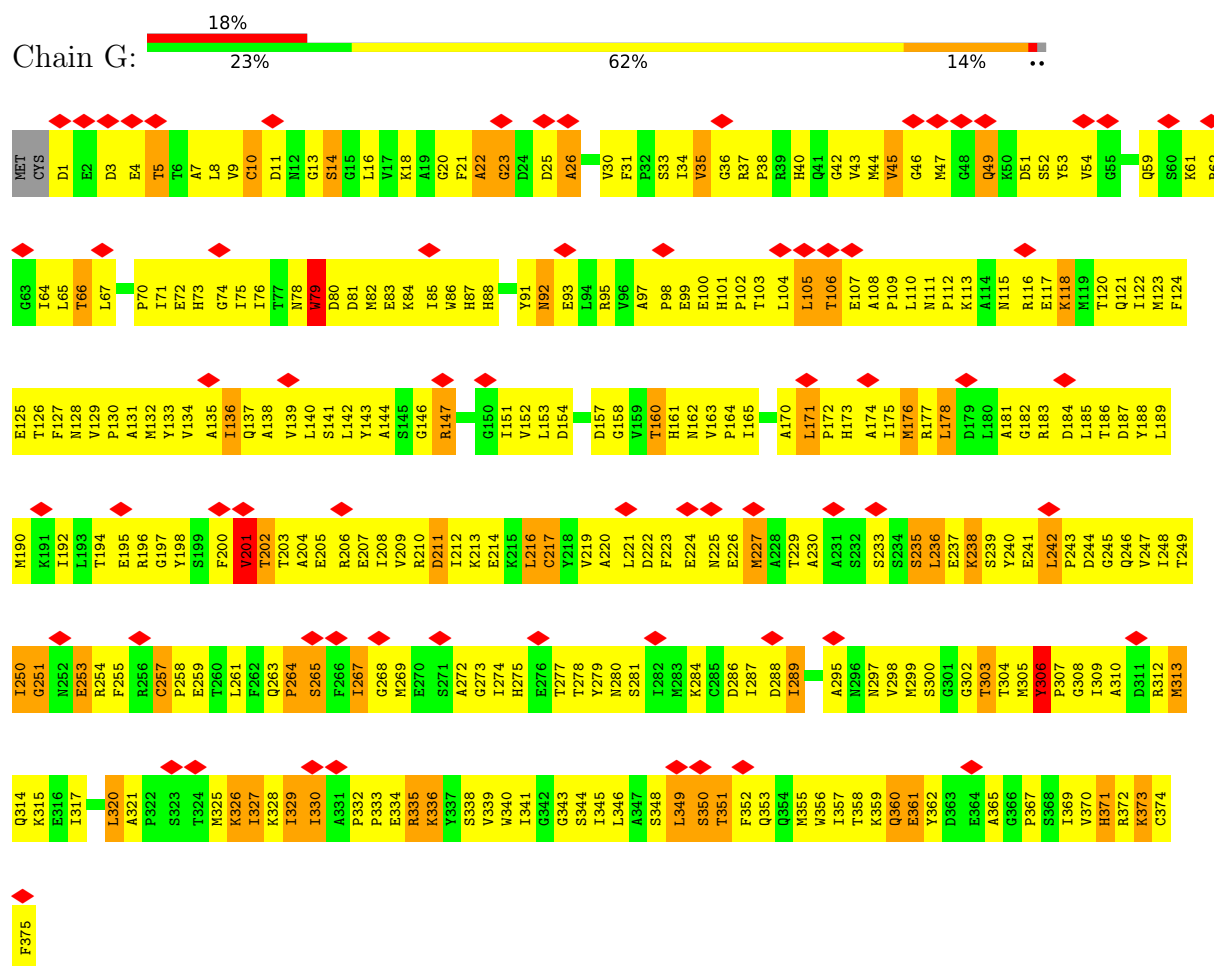




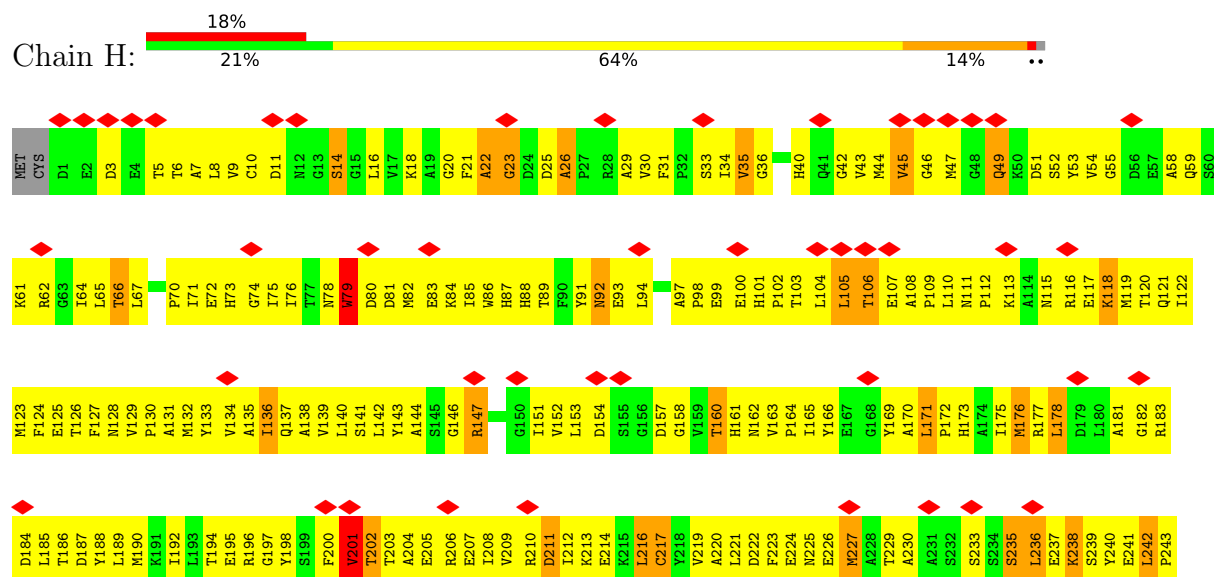
• Molecule 1: Actin, alpha skeletal muscle

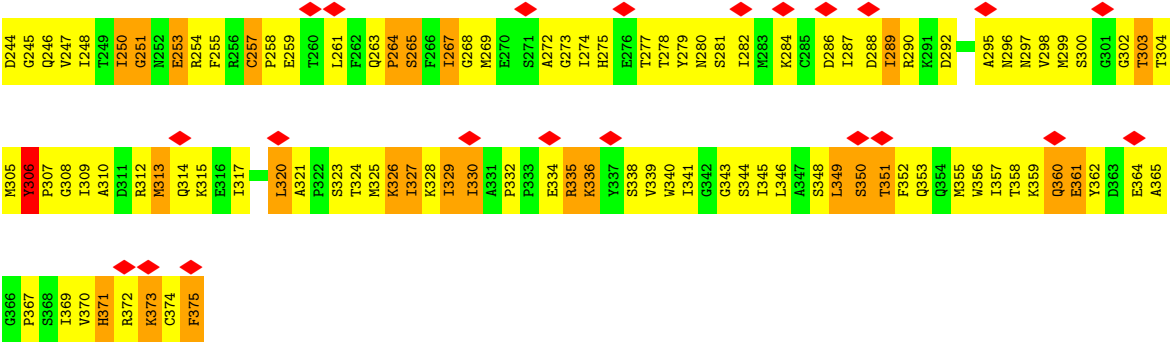


- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=166.7°, rise=27.6 Å, axial sym=C1	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.089	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	168.0, 168.0, 209.99998	wwPDB
Map dimensions	160, 160, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.81	0/2995	0.73	0/4058
1	E	0.81	0/2995	0.72	0/4058
1	F	0.80	0/2995	0.72	0/4058
1	G	0.82	1/2995 (0.0%)	0.72	0/4058
1	H	0.82	1/2995 (0.0%)	0.72	0/4058
All	All	0.81	2/14975 (0.0%)	0.72	0/20290

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	10	CYS	CB-SG	5.58	1.91	1.82
1	H	375	PHE	CE1-CZ	5.04	1.47	1.37

There are no bond angle outliers.

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	D	2932	0	2894	445	0
1	E	2932	0	2894	438	0
1	F	2932	0	2894	475	0
1	G	2932	0	2894	439	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2932	0	2894	450	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	2	0
2	G	27	0	12	2	0
2	H	27	0	12	2	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	14800	0	14530	2165	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 74.

All (2165) 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:H:259:GLU:HB3	1:H:263:GLN:HE22	1.06	1.18
1:E:259:GLU:HB3	1:E:263:GLN:HE22	1.06	1.13
1:G:259:GLU:HB3	1:G:263:GLN:HE22	1.06	1.12
1:F:259:GLU:HB3	1:F:263:GLN:HE22	1.08	1.11
1:D:259:GLU:HB3	1:D:263:GLN:HE22	1.08	1.08
1:H:329:ILE:H	1:H:329:ILE:HD13	1.21	1.02
1:D:329:ILE:HD13	1:D:329:ILE:H	1.23	1.02
1:G:329:ILE:HD13	1:G:329:ILE:H	1.23	1.01
1:E:109:PRO:HD2	1:E:161:HIS:NE2	1.77	1.00
1:D:109:PRO:HD2	1:D:161:HIS:NE2	1.77	1.00
1:E:329:ILE:HD13	1:E:329:ILE:H	1.24	1.00
1:F:329:ILE:H	1:F:329:ILE:HD13	1.27	1.00
1:G:66:THR:HG23	1:G:203:THR:HG21	1.44	0.99
1:E:66:THR:HG23	1:E:203:THR:HG21	1.45	0.99
1:H:109:PRO:HD2	1:H:161:HIS:NE2	1.77	0.99
1:F:147:ARG:HH12	1:F:330:ILE:HD13	1.28	0.98
1:F:109:PRO:HD2	1:F:161:HIS:NE2	1.78	0.98
1:D:66:THR:HG23	1:D:203:THR:HG21	1.42	0.98
1:G:109:PRO:HD2	1:G:161:HIS:NE2	1.77	0.98
1:H:147:ARG:HH12	1:H:330:ILE:HD13	1.29	0.98
1:H:66:THR:HG23	1:H:203:THR:HG21	1.44	0.98
1:E:147:ARG:HH12	1:E:330:ILE:HD13	1.29	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HH12	1:D:330:ILE:HD13	1.28	0.97
1:E:190:MET:HE2	1:E:206:ARG:HG3	1.47	0.97
1:G:147:ARG:HH12	1:G:330:ILE:HD13	1.28	0.96
1:F:76:ILE:H	1:F:115:ASN:HD21	1.11	0.95
1:F:66:THR:HG23	1:F:203:THR:HG21	1.44	0.94
1:G:190:MET:HE2	1:G:206:ARG:HG3	1.51	0.93
1:E:76:ILE:H	1:E:115:ASN:HD21	1.15	0.92
1:G:76:ILE:H	1:G:115:ASN:HD21	1.15	0.92
1:D:76:ILE:H	1:D:115:ASN:HD21	1.14	0.91
1:E:367:PRO:O	1:E:370:VAL:HG12	1.71	0.91
1:F:98:PRO:HB2	1:F:127:PHE:HB3	1.52	0.91
1:G:259:GLU:HB3	1:G:263:GLN:NE2	1.86	0.91
1:E:64:ILE:HD12	1:E:65:LEU:N	1.86	0.91
1:E:259:GLU:HB3	1:E:263:GLN:NE2	1.86	0.91
1:G:64:ILE:HD12	1:G:65:LEU:N	1.86	0.91
1:G:176:MET:HE1	1:G:277:THR:HB	1.53	0.90
1:F:64:ILE:HD12	1:F:65:LEU:N	1.86	0.90
1:D:367:PRO:O	1:D:370:VAL:HG12	1.72	0.90
1:D:136:ILE:HD12	1:D:139:VAL:HG23	1.53	0.90
1:F:202:THR:HG22	1:F:205:GLU:H	1.36	0.90
1:G:238:LYS:HG2	1:G:254:ARG:NH1	1.87	0.90
1:H:76:ILE:H	1:H:115:ASN:HD21	1.14	0.90
1:G:98:PRO:HB2	1:G:127:PHE:HB3	1.53	0.89
1:E:98:PRO:HB2	1:E:127:PHE:HB3	1.52	0.89
1:D:64:ILE:HD12	1:D:65:LEU:N	1.86	0.89
1:G:367:PRO:O	1:G:370:VAL:HG12	1.73	0.89
1:E:202:THR:HG22	1:E:205:GLU:HB2	1.54	0.89
1:H:23:GLY:HA2	1:H:344:SER:HB3	1.52	0.89
1:D:98:PRO:HB2	1:D:127:PHE:HB3	1.53	0.89
1:H:259:GLU:HB3	1:H:263:GLN:NE2	1.87	0.89
1:G:202:THR:HG22	1:G:205:GLU:HB2	1.54	0.88
1:H:64:ILE:HD12	1:H:65:LEU:N	1.88	0.88
1:H:202:THR:HG22	1:H:205:GLU:HB2	1.55	0.88
1:D:259:GLU:HB3	1:D:263:GLN:NE2	1.89	0.88
1:E:202:THR:HG22	1:E:205:GLU:H	1.37	0.88
1:H:98:PRO:HB2	1:H:127:PHE:HB3	1.55	0.88
1:H:238:LYS:HG2	1:H:254:ARG:NH1	1.88	0.88
1:D:190:MET:HE2	1:D:206:ARG:HG3	1.53	0.88
1:E:238:LYS:HG2	1:E:254:ARG:NH1	1.89	0.88
1:G:23:GLY:HA2	1:G:344:SER:HB3	1.55	0.88
1:F:259:GLU:HB3	1:F:263:GLN:NE2	1.89	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:LYS:HG2	1:F:254:ARG:NH1	1.88	0.87
1:H:110:LEU:HB2	1:H:177:ARG:HG3	1.55	0.87
1:D:238:LYS:HG2	1:D:254:ARG:NH1	1.88	0.87
1:H:202:THR:HG22	1:H:205:GLU:H	1.39	0.87
1:H:367:PRO:O	1:H:370:VAL:HG12	1.73	0.87
1:F:71:ILE:HD12	1:F:76:ILE:HG13	1.57	0.87
1:D:202:THR:HG22	1:D:205:GLU:HB2	1.56	0.87
1:D:23:GLY:HA2	1:D:344:SER:HB3	1.55	0.87
1:E:23:GLY:HA2	1:E:344:SER:HB3	1.55	0.87
1:D:110:LEU:HB2	1:D:177:ARG:HG3	1.55	0.86
1:F:23:GLY:HA2	1:F:344:SER:HB3	1.55	0.86
1:H:313:MET:O	1:H:317:ILE:HG12	1.75	0.86
1:G:202:THR:HG22	1:G:205:GLU:H	1.38	0.86
1:D:202:THR:HG22	1:D:205:GLU:H	1.39	0.86
1:E:273:GLY:H	1:E:277:THR:HG23	1.40	0.86
1:F:72:GLU:HA	1:F:183:ARG:HH22	1.41	0.86
1:E:110:LEU:HB2	1:E:177:ARG:HG3	1.56	0.86
1:F:110:LEU:HB2	1:F:177:ARG:HG3	1.56	0.86
1:H:162:ASN:HD21	1:H:278:THR:HG22	1.38	0.86
1:F:136:ILE:HD12	1:F:139:VAL:HG23	1.58	0.86
1:D:72:GLU:HA	1:D:183:ARG:HH22	1.40	0.85
1:H:71:ILE:HD12	1:H:76:ILE:HG13	1.58	0.85
1:F:176:MET:HE1	1:F:277:THR:HB	1.59	0.85
1:G:313:MET:O	1:G:317:ILE:HG12	1.77	0.85
1:G:162:ASN:HD21	1:G:278:THR:HG22	1.40	0.85
1:F:367:PRO:O	1:F:370:VAL:HG12	1.76	0.85
1:E:162:ASN:HD21	1:E:278:THR:HG22	1.41	0.85
1:E:313:MET:O	1:E:317:ILE:HG12	1.75	0.85
1:E:129:VAL:HG21	1:E:132:MET:HG2	1.59	0.85
1:E:136:ILE:HD12	1:E:139:VAL:HG23	1.59	0.85
1:G:72:GLU:HA	1:G:183:ARG:HH22	1.42	0.84
1:G:273:GLY:H	1:G:277:THR:HG23	1.41	0.84
1:H:273:GLY:H	1:H:277:THR:HG23	1.41	0.84
1:E:64:ILE:HD12	1:E:65:LEU:H	1.40	0.84
1:F:162:ASN:HD21	1:F:278:THR:HG22	1.40	0.84
1:F:178:LEU:HD12	1:F:178:LEU:H	1.40	0.84
1:F:202:THR:HG22	1:F:205:GLU:HB2	1.58	0.84
1:D:7:ALA:H	1:D:22:ALA:HB2	1.43	0.84
1:D:313:MET:O	1:D:317:ILE:HG12	1.77	0.84
1:G:110:LEU:HB2	1:G:177:ARG:HG3	1.57	0.84
1:G:136:ILE:HD12	1:G:139:VAL:HG23	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:GLY:H	1:F:277:THR:HG23	1.42	0.84
1:G:8:LEU:O	1:G:103:THR:HA	1.78	0.84
1:F:313:MET:O	1:F:317:ILE:HG12	1.76	0.84
1:H:72:GLU:HA	1:H:183:ARG:HH22	1.41	0.84
1:H:178:LEU:H	1:H:178:LEU:HD12	1.41	0.84
1:E:178:LEU:H	1:E:178:LEU:HD12	1.41	0.84
1:E:71:ILE:HD12	1:E:76:ILE:HG13	1.57	0.83
1:G:178:LEU:H	1:G:178:LEU:HD12	1.42	0.83
1:H:136:ILE:HD12	1:H:139:VAL:HG23	1.60	0.83
1:H:129:VAL:HG21	1:H:132:MET:HG2	1.58	0.83
1:D:273:GLY:H	1:D:277:THR:HG23	1.43	0.83
1:G:71:ILE:HD12	1:G:76:ILE:HG13	1.59	0.83
1:D:71:ILE:HD12	1:D:76:ILE:HG13	1.61	0.83
1:E:8:LEU:O	1:E:103:THR:HA	1.79	0.83
1:F:7:ALA:H	1:F:22:ALA:HB2	1.43	0.83
1:F:129:VAL:HG21	1:F:132:MET:HG2	1.58	0.83
1:H:109:PRO:HG3	1:H:136:ILE:HG12	1.59	0.83
1:D:176:MET:HE1	1:D:277:THR:HB	1.59	0.83
1:D:178:LEU:H	1:D:178:LEU:HD12	1.43	0.82
1:E:72:GLU:HA	1:E:183:ARG:HH22	1.43	0.82
1:D:129:VAL:HG21	1:D:132:MET:HG2	1.59	0.82
1:H:7:ALA:H	1:H:22:ALA:HB2	1.45	0.82
1:E:216:LEU:HD13	1:E:250:ILE:HG12	1.62	0.82
1:F:350:SER:O	1:F:352:PHE:N	2.13	0.82
1:D:169:TYR:HA	1:F:42:GLY:HA3	1.61	0.82
1:E:104:LEU:HD11	1:E:135:ALA:HB2	1.60	0.82
1:F:242:LEU:HD23	1:F:248:ILE:HG23	1.62	0.82
1:D:8:LEU:O	1:D:103:THR:HA	1.79	0.81
1:E:196:ARG:HH21	1:E:251:GLY:HA3	1.45	0.81
1:H:62:ARG:HB3	1:H:204:ALA:HB1	1.61	0.81
1:D:264:PRO:HB2	1:D:269:MET:O	1.79	0.81
1:F:71:ILE:HG13	1:F:75:ILE:O	1.80	0.81
1:G:362:TYR:CE2	1:G:367:PRO:HA	2.15	0.81
1:E:7:ALA:H	1:E:22:ALA:HB2	1.44	0.81
1:G:7:ALA:H	1:G:22:ALA:HB2	1.45	0.81
1:H:196:ARG:HH21	1:H:251:GLY:HA3	1.46	0.81
1:D:104:LEU:HD11	1:D:135:ALA:HB2	1.62	0.81
1:F:169:TYR:HA	1:H:42:GLY:HA3	1.62	0.81
1:D:64:ILE:HD12	1:D:65:LEU:H	1.44	0.81
1:E:242:LEU:HD21	1:E:246:GLN:HB2	1.63	0.81
1:G:129:VAL:HG21	1:G:132:MET:HG2	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:PRO:HB2	1:H:269:MET:O	1.80	0.81
1:D:162:ASN:HD21	1:D:278:THR:HG22	1.43	0.81
1:H:104:LEU:HD11	1:H:135:ALA:HB2	1.62	0.81
1:F:62:ARG:HB3	1:F:204:ALA:HB1	1.62	0.81
1:E:220:ALA:HB1	1:E:226:GLU:HG3	1.63	0.80
1:F:104:LEU:HD11	1:F:135:ALA:HB2	1.63	0.80
1:F:196:ARG:HH21	1:F:251:GLY:HA3	1.47	0.80
1:G:216:LEU:HD13	1:G:250:ILE:HG12	1.64	0.80
1:E:264:PRO:HB2	1:E:269:MET:O	1.80	0.80
1:G:264:PRO:HB2	1:G:269:MET:O	1.81	0.80
1:H:216:LEU:HD13	1:H:250:ILE:HG12	1.62	0.80
1:D:147:ARG:NH1	1:D:330:ILE:HD13	1.97	0.80
1:E:169:TYR:HA	1:G:42:GLY:HA3	1.64	0.80
1:H:8:LEU:O	1:H:103:THR:HA	1.79	0.80
1:H:220:ALA:HB1	1:H:226:GLU:HG3	1.63	0.80
1:G:104:LEU:HD11	1:G:135:ALA:HB2	1.62	0.80
1:F:109:PRO:HG3	1:F:136:ILE:HG12	1.62	0.80
1:E:109:PRO:HG3	1:E:136:ILE:HG12	1.62	0.80
1:F:147:ARG:NH1	1:F:330:ILE:HD13	1.97	0.80
1:E:362:TYR:CE2	1:E:367:PRO:HA	2.17	0.80
1:H:83:GLU:HA	1:H:86:TRP:HE3	1.47	0.80
1:E:176:MET:HE1	1:E:277:THR:HB	1.61	0.80
1:G:242:LEU:HD23	1:G:248:ILE:HG23	1.64	0.80
1:H:71:ILE:HG13	1:H:75:ILE:O	1.82	0.80
1:G:71:ILE:HG13	1:G:75:ILE:O	1.80	0.79
1:E:62:ARG:HB3	1:E:204:ALA:HB1	1.63	0.79
1:G:147:ARG:NH1	1:G:330:ILE:HD13	1.96	0.79
1:D:286:ASP:HB3	1:D:289:ILE:HG22	1.64	0.79
1:H:242:LEU:HD23	1:H:248:ILE:HG23	1.64	0.79
1:D:171:LEU:HD12	1:F:40:HIS:HE1	1.48	0.79
1:H:147:ARG:NH1	1:H:330:ILE:HD13	1.97	0.79
1:D:216:LEU:HD13	1:D:250:ILE:HG12	1.63	0.79
1:F:264:PRO:HB2	1:F:269:MET:O	1.81	0.79
1:G:189:LEU:HD11	1:G:213:LYS:HB3	1.65	0.79
1:D:62:ARG:HB3	1:D:204:ALA:HB1	1.65	0.79
1:E:83:GLU:HA	1:E:86:TRP:HE3	1.48	0.79
1:F:83:GLU:HA	1:F:86:TRP:HE3	1.47	0.79
1:F:189:LEU:HD11	1:F:213:LYS:HB3	1.64	0.79
1:F:216:LEU:HD13	1:F:250:ILE:HG12	1.64	0.79
1:G:196:ARG:HH21	1:G:251:GLY:HA3	1.47	0.79
1:H:242:LEU:HG	1:H:246:GLN:O	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ARG:HB3	1:G:204:ALA:HB1	1.65	0.79
1:F:8:LEU:O	1:F:103:THR:HA	1.82	0.78
1:H:362:TYR:CE2	1:H:367:PRO:HA	2.17	0.78
1:G:109:PRO:HG3	1:G:136:ILE:HG12	1.65	0.78
1:D:350:SER:O	1:D:352:PHE:N	2.16	0.78
1:E:221:LEU:H	1:E:221:LEU:HD12	1.49	0.78
1:F:362:TYR:CE2	1:F:367:PRO:HA	2.18	0.78
1:H:176:MET:HE1	1:H:277:THR:HB	1.64	0.78
1:G:106:THR:HG22	1:G:137:GLN:NE2	1.98	0.78
1:D:242:LEU:HD23	1:D:248:ILE:HG23	1.65	0.78
1:E:286:ASP:HB3	1:E:289:ILE:HG22	1.65	0.78
1:G:362:TYR:HE2	1:G:367:PRO:HA	1.49	0.78
1:E:106:THR:HG22	1:E:137:GLN:NE2	1.98	0.78
1:F:220:ALA:HB1	1:F:226:GLU:HG3	1.65	0.78
1:D:83:GLU:HA	1:D:86:TRP:HE3	1.48	0.78
1:G:83:GLU:HA	1:G:86:TRP:HE3	1.48	0.78
1:H:264:PRO:O	1:H:267:ILE:HG22	1.83	0.78
1:D:196:ARG:HH21	1:D:251:GLY:HA3	1.46	0.78
1:D:362:TYR:CE2	1:D:367:PRO:HA	2.18	0.78
1:E:189:LEU:HD11	1:E:213:LYS:HB3	1.66	0.78
1:D:171:LEU:HD12	1:F:40:HIS:CE1	2.19	0.78
1:F:190:MET:HE2	1:F:206:ARG:HG3	1.65	0.78
1:D:189:LEU:HD11	1:D:213:LYS:HB3	1.66	0.77
1:H:165:ILE:HG13	1:H:170:ALA:CB	2.14	0.77
1:G:242:LEU:HD21	1:G:246:GLN:HB2	1.67	0.77
1:E:71:ILE:HG13	1:E:75:ILE:O	1.83	0.77
1:E:242:LEU:HD23	1:E:248:ILE:HG23	1.67	0.77
1:H:165:ILE:HG13	1:H:170:ALA:HB2	1.65	0.77
1:E:147:ARG:NH1	1:E:330:ILE:HD13	1.98	0.77
1:G:350:SER:O	1:G:352:PHE:N	2.18	0.77
1:H:189:LEU:HD11	1:H:213:LYS:HB3	1.65	0.77
1:H:190:MET:HE2	1:H:206:ARG:HG3	1.65	0.77
1:E:362:TYR:HE2	1:E:367:PRO:HA	1.50	0.77
1:G:64:ILE:HD12	1:G:65:LEU:H	1.47	0.77
1:H:64:ILE:HD12	1:H:65:LEU:H	1.49	0.77
1:H:286:ASP:HB3	1:H:289:ILE:HG22	1.67	0.77
1:D:109:PRO:HG3	1:D:136:ILE:HG12	1.65	0.77
1:G:154:ASP:OD1	1:G:161:HIS:HB2	1.85	0.76
1:H:106:THR:HG22	1:H:137:GLN:NE2	1.99	0.76
1:H:242:LEU:HD21	1:H:246:GLN:HB2	1.66	0.76
1:D:154:ASP:OD1	1:D:161:HIS:HB2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:LEU:HD21	1:F:246:GLN:HB2	1.66	0.76
1:F:64:ILE:HD12	1:F:65:LEU:H	1.49	0.76
1:E:154:ASP:OD1	1:E:161:HIS:HB2	1.85	0.76
1:G:220:ALA:HB1	1:G:226:GLU:HG3	1.66	0.76
1:H:362:TYR:HE2	1:H:367:PRO:HA	1.50	0.75
1:H:99:GLU:HG3	1:H:128:ASN:HB2	1.69	0.75
1:D:242:LEU:HD21	1:D:246:GLN:HB2	1.67	0.75
1:F:106:THR:HG22	1:F:137:GLN:NE2	2.00	0.75
1:G:286:ASP:HB3	1:G:289:ILE:HG22	1.67	0.75
1:E:242:LEU:HG	1:E:246:GLN:O	1.87	0.75
1:G:165:ILE:HG13	1:G:170:ALA:HB2	1.67	0.75
1:D:220:ALA:HB1	1:D:226:GLU:HG3	1.69	0.75
1:F:237:GLU:O	1:F:238:LYS:HG3	1.86	0.75
1:F:286:ASP:HB3	1:F:289:ILE:HG22	1.68	0.75
1:G:237:GLU:O	1:G:238:LYS:HG3	1.87	0.75
1:G:242:LEU:HG	1:G:246:GLN:O	1.86	0.75
1:D:71:ILE:HG13	1:D:75:ILE:O	1.85	0.75
1:G:264:PRO:O	1:G:267:ILE:HG22	1.87	0.75
1:F:99:GLU:HG3	1:F:128:ASN:HB2	1.69	0.74
1:G:105:LEU:HD21	1:G:132:MET:HB2	1.69	0.74
1:H:221:LEU:H	1:H:221:LEU:HD12	1.52	0.74
1:F:83:GLU:HA	1:F:86:TRP:CE3	2.23	0.74
1:H:154:ASP:OD1	1:H:161:HIS:HB2	1.86	0.74
1:H:238:LYS:NZ	1:H:254:ARG:HH22	1.86	0.74
1:H:83:GLU:HA	1:H:86:TRP:CE3	2.22	0.74
1:E:171:LEU:HD12	1:G:40:HIS:HE1	1.52	0.74
1:F:362:TYR:HE2	1:F:367:PRO:HA	1.52	0.74
1:H:141:SER:HA	1:H:338:SER:HB2	1.70	0.74
1:E:171:LEU:HD12	1:G:40:HIS:CE1	2.23	0.74
1:E:350:SER:O	1:E:352:PHE:N	2.20	0.74
1:D:106:THR:HG22	1:D:137:GLN:NE2	2.01	0.74
1:E:165:ILE:HG13	1:E:170:ALA:HB2	1.70	0.74
1:E:105:LEU:HD21	1:E:132:MET:HB2	1.70	0.74
1:H:81:ASP:O	1:H:84:LYS:HG2	1.87	0.74
1:D:303:THR:O	1:D:306:TYR:HB2	1.88	0.73
1:F:154:ASP:OD1	1:F:161:HIS:HB2	1.88	0.73
1:G:112:PRO:HG3	1:H:197:GLY:HA2	1.68	0.73
1:D:81:ASP:O	1:D:84:LYS:HG2	1.88	0.73
1:D:362:TYR:HE2	1:D:367:PRO:HA	1.53	0.73
1:F:105:LEU:HD21	1:F:132:MET:HB2	1.70	0.73
1:F:171:LEU:HD12	1:H:40:HIS:HE1	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LEU:HD21	1:H:132:MET:HB2	1.70	0.73
1:D:83:GLU:HA	1:D:86:TRP:CE3	2.23	0.73
1:E:99:GLU:HG3	1:E:128:ASN:HB2	1.69	0.73
1:E:165:ILE:HG13	1:E:170:ALA:CB	2.18	0.73
1:G:83:GLU:HA	1:G:86:TRP:CE3	2.23	0.73
1:E:83:GLU:HA	1:E:86:TRP:CE3	2.23	0.73
1:H:350:SER:O	1:H:352:PHE:N	2.21	0.73
1:D:105:LEU:HD21	1:D:132:MET:HB2	1.71	0.73
1:G:141:SER:HA	1:G:338:SER:HB2	1.71	0.73
1:G:165:ILE:HG13	1:G:170:ALA:CB	2.18	0.73
1:G:258:PRO:HG3	1:G:306:TYR:HE2	1.53	0.73
1:D:238:LYS:NZ	1:D:254:ARG:HH22	1.87	0.72
1:F:112:PRO:HG3	1:G:197:GLY:HA2	1.69	0.72
1:H:258:PRO:HG3	1:H:306:TYR:HE2	1.54	0.72
1:D:221:LEU:H	1:D:221:LEU:HD12	1.55	0.72
1:D:258:PRO:HG3	1:D:306:TYR:HE2	1.55	0.72
1:D:264:PRO:O	1:D:267:ILE:HG22	1.89	0.72
1:F:171:LEU:HD12	1:H:40:HIS:CE1	2.24	0.72
1:F:221:LEU:HD12	1:F:221:LEU:H	1.55	0.72
1:G:33:SER:HB2	1:G:85:ILE:HD13	1.71	0.72
1:E:81:ASP:O	1:E:84:LYS:HG2	1.90	0.72
1:D:165:ILE:HG13	1:D:170:ALA:HB2	1.72	0.72
1:D:141:SER:HA	1:D:338:SER:HB2	1.70	0.72
1:D:171:LEU:HA	1:F:40:HIS:NE2	2.05	0.72
1:F:258:PRO:HG3	1:F:306:TYR:HE2	1.55	0.72
1:F:303:THR:O	1:F:306:TYR:HB2	1.90	0.72
1:D:99:GLU:HG3	1:D:128:ASN:HB2	1.72	0.71
1:H:152:VAL:HG12	1:H:298:VAL:HG13	1.70	0.71
1:D:165:ILE:HG13	1:D:170:ALA:CB	2.20	0.71
1:E:33:SER:HB2	1:E:85:ILE:HD13	1.72	0.71
1:E:46:GLY:H	1:E:49:GLN:HB2	1.54	0.71
1:F:264:PRO:O	1:F:267:ILE:HG22	1.90	0.71
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.71	0.71
1:F:165:ILE:HG13	1:F:170:ALA:CB	2.20	0.71
1:E:152:VAL:HG12	1:E:298:VAL:HG13	1.71	0.71
1:E:237:GLU:O	1:E:238:LYS:HG3	1.90	0.71
1:G:221:LEU:H	1:G:221:LEU:HD12	1.56	0.71
1:H:124:PHE:CZ	1:H:362:TYR:HB3	2.26	0.71
1:E:141:SER:HA	1:E:338:SER:HB2	1.72	0.71
1:F:81:ASP:O	1:F:84:LYS:HG2	1.89	0.71
1:H:310:ALA:HB1	1:H:329:ILE:HG13	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLU:O	1:D:238:LYS:HG3	1.91	0.71
1:F:217:CYS:SG	1:F:307:PRO:HD2	2.31	0.71
1:G:81:ASP:O	1:G:84:LYS:HG2	1.90	0.71
1:H:33:SER:HB2	1:H:85:ILE:HD13	1.71	0.71
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.72	0.71
1:H:219:VAL:HG21	1:H:308:GLY:O	1.90	0.71
1:F:76:ILE:H	1:F:115:ASN:ND2	1.87	0.71
1:F:350:SER:C	1:F:352:PHE:H	1.94	0.71
1:G:310:ALA:HB1	1:G:329:ILE:HG13	1.72	0.71
1:G:219:VAL:HG21	1:G:308:GLY:O	1.91	0.71
1:H:217:CYS:SG	1:H:307:PRO:HD2	2.31	0.70
1:D:242:LEU:HG	1:D:246:GLN:O	1.92	0.70
1:H:54:VAL:HG21	1:H:88:HIS:CG	2.27	0.70
1:E:54:VAL:HG21	1:E:88:HIS:CG	2.26	0.70
1:F:157:ASP:O	1:F:183:ARG:HB3	1.92	0.70
1:G:59:GLN:O	1:G:62:ARG:HG3	1.91	0.70
1:G:238:LYS:NZ	1:G:254:ARG:HH22	1.88	0.70
1:D:46:GLY:H	1:D:49:GLN:HB2	1.56	0.70
1:E:76:ILE:H	1:E:115:ASN:ND2	1.89	0.70
1:E:203:THR:O	1:E:207:GLU:HG2	1.92	0.70
1:E:217:CYS:SG	1:E:307:PRO:HD2	2.32	0.70
1:F:264:PRO:HD2	1:F:272:ALA:O	1.92	0.70
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.73	0.70
1:D:302:GLY:C	1:D:304:THR:H	1.95	0.70
1:F:33:SER:HB2	1:F:85:ILE:HD13	1.72	0.70
1:G:203:THR:O	1:G:207:GLU:HG2	1.92	0.70
1:E:152:VAL:HG12	1:E:298:VAL:CG1	2.21	0.70
1:H:71:ILE:HD11	1:H:74:GLY:C	2.12	0.70
1:H:230:ALA:HB1	1:H:236:LEU:HD21	1.73	0.70
1:D:297:ASN:HB3	1:D:328:LYS:O	1.92	0.70
1:E:59:GLN:O	1:E:62:ARG:HG3	1.92	0.70
1:E:171:LEU:HA	1:G:40:HIS:NE2	2.05	0.70
1:F:118:LYS:HA	1:F:118:LYS:HE2	1.74	0.70
1:F:124:PHE:CZ	1:F:362:TYR:HB3	2.27	0.70
1:F:242:LEU:HG	1:F:246:GLN:O	1.92	0.70
1:F:310:ALA:HB1	1:F:329:ILE:HG13	1.72	0.70
1:D:109:PRO:O	1:D:177:ARG:HD3	1.91	0.70
1:D:152:VAL:HG12	1:D:298:VAL:HG13	1.72	0.70
1:E:264:PRO:O	1:E:267:ILE:HG22	1.92	0.70
1:F:152:VAL:HG12	1:F:298:VAL:HG13	1.72	0.70
1:F:165:ILE:HG13	1:F:170:ALA:HB2	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:PHE:CZ	1:D:362:TYR:HB3	2.27	0.69
1:D:310:ALA:HB1	1:D:329:ILE:HG13	1.73	0.69
1:E:124:PHE:CZ	1:E:362:TYR:HB3	2.26	0.69
1:G:71:ILE:HD11	1:G:74:GLY:C	2.12	0.69
1:G:152:VAL:HG12	1:G:298:VAL:HG13	1.73	0.69
1:E:118:LYS:HE2	1:E:118:LYS:HA	1.72	0.69
1:F:238:LYS:NZ	1:F:254:ARG:HH22	1.89	0.69
1:H:152:VAL:HG12	1:H:298:VAL:CG1	2.20	0.69
1:E:238:LYS:NZ	1:E:254:ARG:HH22	1.88	0.69
1:F:141:SER:HA	1:F:338:SER:HB2	1.74	0.69
1:H:237:GLU:O	1:H:238:LYS:HG3	1.92	0.69
1:D:136:ILE:CD1	1:D:139:VAL:H	2.05	0.69
1:D:238:LYS:HZ2	1:D:254:ARG:HH22	1.41	0.69
1:E:236:LEU:HD13	1:E:236:LEU:H	1.57	0.69
1:F:230:ALA:HB1	1:F:236:LEU:HD21	1.75	0.69
1:G:302:GLY:C	1:G:304:THR:H	1.96	0.69
1:H:136:ILE:CD1	1:H:139:VAL:H	2.06	0.69
1:H:203:THR:O	1:H:207:GLU:HG2	1.93	0.69
1:E:340:TRP:HE3	1:E:341:ILE:HD13	1.57	0.69
1:G:46:GLY:H	1:G:49:GLN:HB2	1.57	0.69
1:H:59:GLN:O	1:H:62:ARG:HG3	1.92	0.69
1:E:112:PRO:HG3	1:F:197:GLY:HA2	1.73	0.69
1:G:99:GLU:HG3	1:G:128:ASN:HB2	1.73	0.69
1:H:303:THR:O	1:H:306:TYR:HB2	1.93	0.69
1:D:329:ILE:H	1:D:329:ILE:CD1	2.02	0.69
1:D:59:GLN:O	1:D:62:ARG:HG3	1.93	0.69
1:D:76:ILE:H	1:D:115:ASN:ND2	1.89	0.69
1:D:112:PRO:HG3	1:E:197:GLY:HA2	1.73	0.69
1:E:303:THR:O	1:E:306:TYR:HB2	1.92	0.69
1:F:59:GLN:O	1:F:62:ARG:HG3	1.92	0.69
1:F:136:ILE:CD1	1:F:139:VAL:H	2.06	0.69
1:F:219:VAL:HG21	1:F:308:GLY:O	1.92	0.69
1:G:303:THR:O	1:G:306:TYR:HB2	1.92	0.69
1:H:118:LYS:HE2	1:H:118:LYS:HA	1.75	0.69
1:E:124:PHE:HA	1:E:129:VAL:HG22	1.75	0.69
1:F:190:MET:CE	1:F:206:ARG:HG3	2.23	0.69
1:D:33:SER:HB2	1:D:85:ILE:HD13	1.73	0.69
1:F:54:VAL:HG21	1:F:88:HIS:CG	2.28	0.69
1:F:203:THR:O	1:F:207:GLU:HG2	1.93	0.69
1:H:221:LEU:HB3	1:H:315:LYS:HE2	1.73	0.69
1:D:226:GLU:HA	1:D:229:THR:HG22	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ALA:HB1	1:D:236:LEU:HD21	1.75	0.68
1:E:310:ALA:HB1	1:E:329:ILE:HG13	1.73	0.68
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.73	0.68
1:G:106:THR:HG22	1:G:137:GLN:HE22	1.58	0.68
1:G:264:PRO:HD2	1:G:272:ALA:O	1.92	0.68
1:D:152:VAL:HG12	1:D:298:VAL:CG1	2.22	0.68
1:E:157:ASP:O	1:E:183:ARG:HB3	1.94	0.68
1:F:297:ASN:HB3	1:F:328:LYS:O	1.94	0.68
1:F:302:GLY:C	1:F:304:THR:H	1.96	0.68
1:G:54:VAL:HG21	1:G:88:HIS:CG	2.28	0.68
1:H:190:MET:CE	1:H:206:ARG:HG3	2.23	0.68
1:H:302:GLY:C	1:H:304:THR:H	1.95	0.68
1:E:258:PRO:HG3	1:E:306:TYR:HE2	1.56	0.68
1:F:171:LEU:HA	1:H:40:HIS:NE2	2.08	0.68
1:G:79:TRP:HA	1:G:79:TRP:CE3	2.29	0.68
1:E:106:THR:HG22	1:E:137:GLN:HE22	1.58	0.68
1:E:136:ILE:CD1	1:E:139:VAL:H	2.06	0.68
1:G:340:TRP:HE3	1:G:341:ILE:HD13	1.58	0.68
1:H:340:TRP:HE3	1:H:341:ILE:HD13	1.57	0.68
1:E:330:ILE:O	1:E:330:ILE:HG22	1.94	0.68
1:G:302:GLY:O	1:G:304:THR:N	2.27	0.68
1:H:79:TRP:CE3	1:H:79:TRP:HA	2.29	0.68
1:D:203:THR:O	1:D:207:GLU:HG2	1.94	0.68
1:G:136:ILE:CD1	1:G:139:VAL:H	2.05	0.68
1:H:46:GLY:H	1:H:49:GLN:HB2	1.58	0.68
1:F:152:VAL:HG12	1:F:298:VAL:CG1	2.23	0.68
1:D:327:ILE:HD13	1:D:327:ILE:H	1.58	0.68
1:D:330:ILE:HG22	1:D:330:ILE:O	1.93	0.68
1:H:76:ILE:H	1:H:115:ASN:ND2	1.90	0.68
1:D:124:PHE:HA	1:D:129:VAL:HG22	1.75	0.68
1:G:152:VAL:HG12	1:G:298:VAL:CG1	2.24	0.68
1:H:329:ILE:HD13	1:H:329:ILE:N	2.03	0.68
1:E:297:ASN:HB3	1:E:328:LYS:O	1.93	0.68
1:E:302:GLY:C	1:E:304:THR:H	1.97	0.68
1:F:340:TRP:HE3	1:F:341:ILE:HD13	1.57	0.68
1:D:91:TYR:O	1:D:92:ASN:CB	2.42	0.67
1:G:124:PHE:CZ	1:G:362:TYR:HB3	2.28	0.67
1:G:217:CYS:SG	1:G:307:PRO:HD2	2.34	0.67
1:E:230:ALA:HB1	1:E:236:LEU:HD21	1.76	0.67
1:G:230:ALA:HB1	1:G:236:LEU:HD21	1.76	0.67
1:D:71:ILE:HD11	1:D:74:GLY:C	2.14	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:VAL:HG21	1:D:308:GLY:O	1.93	0.67
1:D:340:TRP:HE3	1:D:341:ILE:HD13	1.58	0.67
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.76	0.67
1:E:221:LEU:HB3	1:E:315:LYS:HE2	1.77	0.67
1:F:236:LEU:H	1:F:236:LEU:HD13	1.60	0.67
1:F:238:LYS:HG2	1:F:254:ARG:HH12	1.60	0.67
1:D:54:VAL:HG21	1:D:88:HIS:CG	2.29	0.67
1:G:124:PHE:HA	1:G:129:VAL:HG22	1.77	0.67
1:G:202:THR:CG2	1:G:205:GLU:H	2.08	0.67
1:G:352:PHE:O	1:G:355:MET:HG2	1.94	0.67
1:H:297:ASN:HB3	1:H:328:LYS:O	1.95	0.67
1:F:273:GLY:O	1:F:277:THR:HG23	1.94	0.67
1:G:350:SER:C	1:G:352:PHE:H	1.98	0.67
1:F:219:VAL:HG13	1:F:307:PRO:O	1.95	0.67
1:G:190:MET:CE	1:G:206:ARG:HG3	2.22	0.67
1:G:327:ILE:HD13	1:G:327:ILE:H	1.59	0.67
1:G:330:ILE:O	1:G:330:ILE:HG22	1.95	0.67
1:H:362:TYR:O	1:H:365:ALA:O	2.13	0.67
1:D:264:PRO:HD2	1:D:272:ALA:O	1.95	0.67
1:D:350:SER:C	1:D:352:PHE:H	1.98	0.67
1:E:78:ASN:HB3	1:E:81:ASP:OD2	1.95	0.67
1:F:71:ILE:HD11	1:F:74:GLY:C	2.16	0.67
1:G:76:ILE:H	1:G:115:ASN:ND2	1.90	0.67
1:D:78:ASN:HB3	1:D:81:ASP:OD2	1.95	0.66
1:F:124:PHE:HA	1:F:129:VAL:HG22	1.77	0.66
1:F:291:LYS:HB2	1:H:244:ASP:OD2	1.95	0.66
1:G:219:VAL:HG13	1:G:307:PRO:O	1.95	0.66
1:D:217:CYS:SG	1:D:307:PRO:HD2	2.35	0.66
1:E:190:MET:CE	1:E:206:ARG:HG3	2.22	0.66
1:E:219:VAL:HG21	1:E:308:GLY:O	1.95	0.66
1:G:118:LYS:HE2	1:G:118:LYS:HA	1.75	0.66
1:H:106:THR:HG22	1:H:137:GLN:HE22	1.59	0.66
1:D:118:LYS:HE2	1:D:118:LYS:HA	1.77	0.66
1:D:171:LEU:HA	1:F:40:HIS:HE2	1.61	0.66
1:E:71:ILE:HD11	1:E:74:GLY:C	2.15	0.66
1:E:143:TYR:CZ	1:G:44:MET:SD	2.88	0.66
1:E:264:PRO:HD2	1:E:272:ALA:O	1.95	0.66
1:F:170:ALA:O	1:H:40:HIS:NE2	2.28	0.66
1:D:157:ASP:O	1:D:183:ARG:HB3	1.95	0.66
1:D:170:ALA:O	1:F:40:HIS:NE2	2.29	0.66
1:D:273:GLY:O	1:D:277:THR:HG23	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ILE:HD13	1:D:329:ILE:N	2.06	0.66
1:F:143:TYR:CZ	1:H:44:MET:SD	2.89	0.66
1:F:221:LEU:HB3	1:F:315:LYS:HE2	1.76	0.66
1:F:362:TYR:O	1:F:365:ALA:O	2.14	0.66
1:H:202:THR:CG2	1:H:205:GLU:H	2.09	0.66
1:D:219:VAL:HG13	1:D:307:PRO:O	1.96	0.66
1:E:52:SER:HB2	1:E:65:LEU:HD13	1.77	0.66
1:G:113:LYS:HE2	1:H:195:GLU:HG3	1.77	0.66
1:H:110:LEU:HD11	1:H:175:ILE:HB	1.76	0.66
1:E:255:PHE:O	1:E:258:PRO:HD2	1.96	0.66
1:E:352:PHE:O	1:E:355:MET:HG2	1.95	0.66
1:H:154:ASP:HA	1:H:300:SER:O	1.95	0.66
1:H:302:GLY:O	1:H:304:THR:N	2.26	0.66
1:D:79:TRP:HA	1:D:79:TRP:CE3	2.30	0.65
1:D:190:MET:CE	1:D:206:ARG:HG3	2.26	0.65
1:F:46:GLY:H	1:F:49:GLN:HB2	1.59	0.65
1:H:109:PRO:O	1:H:177:ARG:HD3	1.96	0.65
1:F:78:ASN:HB3	1:F:81:ASP:OD2	1.96	0.65
1:G:157:ASP:O	1:G:183:ARG:HB3	1.96	0.65
1:H:330:ILE:O	1:H:330:ILE:HG22	1.96	0.65
1:H:350:SER:C	1:H:352:PHE:H	2.00	0.65
1:E:273:GLY:O	1:E:277:THR:HG23	1.96	0.65
1:G:78:ASN:HB3	1:G:81:ASP:OD2	1.96	0.65
1:H:236:LEU:H	1:H:236:LEU:HD13	1.60	0.65
1:F:113:LYS:HE2	1:G:195:GLU:HG3	1.78	0.65
1:G:109:PRO:O	1:G:177:ARG:HD3	1.96	0.65
1:H:274:ILE:HA	1:H:277:THR:OG1	1.96	0.65
1:D:107:GLU:OE2	1:D:116:ARG:HG2	1.97	0.65
1:F:7:ALA:O	1:F:22:ALA:N	2.30	0.65
1:F:176:MET:CE	1:F:277:THR:HB	2.27	0.65
1:H:257:CYS:SG	1:H:258:PRO:HD3	2.36	0.65
1:H:273:GLY:O	1:H:277:THR:HG23	1.96	0.65
1:E:79:TRP:CE3	1:E:79:TRP:HA	2.30	0.65
1:E:110:LEU:HD11	1:E:175:ILE:HB	1.79	0.65
1:G:71:ILE:HG13	1:G:75:ILE:C	2.17	0.65
1:D:221:LEU:HB3	1:D:315:LYS:HE2	1.77	0.65
1:E:202:THR:CG2	1:E:205:GLU:H	2.07	0.65
1:E:302:GLY:O	1:E:304:THR:N	2.30	0.65
1:F:98:PRO:CB	1:F:127:PHE:HB3	2.27	0.65
1:E:107:GLU:OE2	1:E:116:ARG:HG2	1.97	0.65
1:G:297:ASN:HB3	1:G:328:LYS:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:PHE:HA	1:H:129:VAL:HG22	1.78	0.65
1:D:72:GLU:HA	1:D:183:ARG:NH2	2.11	0.65
1:E:327:ILE:H	1:E:327:ILE:HD13	1.62	0.65
1:F:274:ILE:HA	1:F:277:THR:OG1	1.97	0.65
1:G:157:ASP:C	1:G:181:ALA:HB1	2.17	0.65
1:G:362:TYR:O	1:G:365:ALA:O	2.15	0.65
1:H:264:PRO:HD2	1:H:272:ALA:O	1.97	0.65
1:D:143:TYR:CZ	1:F:44:MET:SD	2.90	0.64
1:D:176:MET:CE	1:D:277:THR:HB	2.27	0.64
1:E:279:TYR:CD2	1:E:320:LEU:HD13	2.32	0.64
1:H:78:ASN:HB3	1:H:81:ASP:OD2	1.97	0.64
1:F:302:GLY:O	1:F:304:THR:N	2.29	0.64
1:F:327:ILE:HD13	1:F:327:ILE:H	1.61	0.64
1:H:261:LEU:O	1:H:274:ILE:HG12	1.97	0.64
1:F:329:ILE:HD13	1:F:329:ILE:N	2.08	0.64
1:H:219:VAL:HG13	1:H:307:PRO:O	1.96	0.64
1:E:273:GLY:O	1:E:277:THR:N	2.25	0.64
1:E:349:LEU:HB3	1:E:352:PHE:CE2	2.32	0.64
1:G:273:GLY:O	1:G:277:THR:HG23	1.97	0.64
1:E:147:ARG:HH22	1:E:330:ILE:CD1	2.11	0.64
1:E:170:ALA:O	1:G:40:HIS:NE2	2.31	0.64
1:F:107:GLU:OE2	1:F:116:ARG:HG2	1.97	0.64
1:F:147:ARG:HH22	1:F:330:ILE:CD1	2.11	0.64
1:F:154:ASP:HA	1:F:300:SER:O	1.98	0.64
1:F:157:ASP:C	1:F:181:ALA:HB1	2.17	0.64
1:H:273:GLY:O	1:H:277:THR:N	2.27	0.64
1:D:210:ARG:O	1:D:211:ASP:HB3	1.98	0.64
1:G:91:TYR:O	1:G:92:ASN:CB	2.46	0.64
1:H:327:ILE:H	1:H:327:ILE:HD13	1.61	0.64
1:D:52:SER:HB2	1:D:65:LEU:HD13	1.78	0.64
1:D:136:ILE:HG23	1:D:139:VAL:HB	1.80	0.64
1:D:240:TYR:CE1	1:D:241:GLU:O	2.51	0.64
1:E:157:ASP:C	1:E:181:ALA:HB1	2.17	0.64
1:H:157:ASP:O	1:H:183:ARG:HB3	1.98	0.64
1:E:350:SER:C	1:E:352:PHE:H	2.01	0.64
1:F:79:TRP:HA	1:F:79:TRP:CE3	2.32	0.64
1:H:329:ILE:H	1:H:329:ILE:CD1	2.01	0.64
1:E:171:LEU:HA	1:G:40:HIS:HE2	1.63	0.64
1:F:330:ILE:HG22	1:F:330:ILE:O	1.96	0.64
1:F:352:PHE:O	1:F:355:MET:HG2	1.97	0.64
1:G:7:ALA:O	1:G:22:ALA:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ARG:HH22	1:G:330:ILE:CD1	2.10	0.64
1:G:210:ARG:O	1:G:211:ASP:HB3	1.98	0.64
1:E:182:GLY:O	1:E:185:LEU:HB3	1.98	0.64
1:F:106:THR:HG22	1:F:137:GLN:HE22	1.62	0.64
1:H:212:ILE:HG22	1:H:216:LEU:HD12	1.80	0.64
1:H:255:PHE:O	1:H:258:PRO:HD2	1.97	0.64
1:D:147:ARG:HH22	1:D:330:ILE:CD1	2.11	0.63
1:E:7:ALA:O	1:E:22:ALA:N	2.30	0.63
1:E:109:PRO:O	1:E:177:ARG:HD3	1.97	0.63
1:E:154:ASP:HA	1:E:300:SER:O	1.98	0.63
1:G:110:LEU:HD11	1:G:175:ILE:HB	1.80	0.63
1:H:157:ASP:C	1:H:181:ALA:HB1	2.17	0.63
1:H:176:MET:CE	1:H:277:THR:HB	2.28	0.63
1:H:238:LYS:HG2	1:H:254:ARG:HH12	1.61	0.63
1:D:222:ASP:O	1:D:224:GLU:N	2.31	0.63
1:D:302:GLY:O	1:D:304:THR:N	2.28	0.63
1:G:176:MET:CE	1:G:277:THR:HB	2.27	0.63
1:H:113:LYS:HG2	1:H:117:GLU:OE1	1.98	0.63
1:D:291:LYS:HB2	1:F:244:ASP:OD2	1.99	0.63
1:E:113:LYS:HE2	1:F:195:GLU:HG3	1.79	0.63
1:E:261:LEU:O	1:E:274:ILE:HG12	1.99	0.63
1:G:221:LEU:HB3	1:G:315:LYS:HE2	1.80	0.63
1:G:236:LEU:HD13	1:G:236:LEU:H	1.64	0.63
1:D:202:THR:CG2	1:D:205:GLU:H	2.09	0.63
1:F:110:LEU:HD11	1:F:175:ILE:HB	1.79	0.63
1:F:171:LEU:HA	1:H:40:HIS:HE2	1.64	0.63
1:F:172:PRO:HA	1:F:175:ILE:HD11	1.79	0.63
1:G:52:SER:HB2	1:G:65:LEU:HD13	1.79	0.63
1:G:261:LEU:O	1:G:274:ILE:HG12	1.98	0.63
1:G:274:ILE:HA	1:G:277:THR:OG1	1.98	0.63
1:H:62:ARG:HB3	1:H:204:ALA:CB	2.28	0.63
1:H:72:GLU:HA	1:H:183:ARG:NH2	2.12	0.63
1:H:202:THR:HG22	1:H:205:GLU:CB	2.28	0.63
1:D:279:TYR:CD2	1:D:320:LEU:HD13	2.34	0.63
1:D:212:ILE:HG22	1:D:216:LEU:HD12	1.81	0.63
1:F:72:GLU:HA	1:F:183:ARG:NH2	2.12	0.63
1:G:107:GLU:OE2	1:G:116:ARG:HG2	1.98	0.63
1:D:157:ASP:C	1:D:181:ALA:HB1	2.19	0.63
1:E:176:MET:CE	1:E:277:THR:HB	2.28	0.63
1:E:202:THR:HG22	1:E:205:GLU:CB	2.27	0.63
1:F:91:TYR:O	1:F:92:ASN:CB	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:ILE:HG22	1:G:216:LEU:HD12	1.80	0.63
1:E:210:ARG:O	1:E:211:ASP:HB3	1.99	0.63
1:H:109:PRO:CG	1:H:136:ILE:HG12	2.29	0.63
1:D:238:LYS:HG2	1:D:254:ARG:HH12	1.62	0.62
1:H:107:GLU:OE2	1:H:116:ARG:HG2	1.97	0.62
1:E:113:LYS:HG2	1:E:117:GLU:OE1	1.99	0.62
1:F:212:ILE:HG22	1:F:216:LEU:HD12	1.81	0.62
1:F:240:TYR:CE1	1:F:241:GLU:O	2.53	0.62
1:G:72:GLU:HA	1:G:183:ARG:NH2	2.13	0.62
1:G:329:ILE:H	1:G:329:ILE:CD1	2.03	0.62
1:H:91:TYR:O	1:H:92:ASN:CB	2.47	0.62
1:E:71:ILE:HG13	1:E:75:ILE:C	2.20	0.62
1:E:291:LYS:HB2	1:G:244:ASP:OD2	1.98	0.62
1:F:349:LEU:HB3	1:F:352:PHE:CE2	2.33	0.62
1:D:7:ALA:O	1:D:22:ALA:N	2.32	0.62
1:F:122:ILE:O	1:F:126:THR:HB	1.99	0.62
1:G:172:PRO:HA	1:G:175:ILE:HD11	1.81	0.62
1:H:349:LEU:HB3	1:H:352:PHE:CE2	2.33	0.62
1:H:352:PHE:O	1:H:355:MET:HG2	1.98	0.62
1:D:71:ILE:HG13	1:D:75:ILE:C	2.20	0.62
1:D:106:THR:HG22	1:D:137:GLN:HE22	1.62	0.62
1:D:182:GLY:O	1:D:185:LEU:HB3	1.99	0.62
1:E:212:ILE:HG22	1:E:216:LEU:HD12	1.81	0.62
1:F:202:THR:CG2	1:F:205:GLU:H	2.08	0.62
1:F:227:MET:HA	1:F:255:PHE:HZ	1.64	0.62
1:E:219:VAL:HG13	1:E:307:PRO:O	1.99	0.62
1:F:113:LYS:HG2	1:F:117:GLU:OE1	1.99	0.62
1:F:209:VAL:O	1:F:212:ILE:HG12	1.98	0.62
1:G:202:THR:HG22	1:G:205:GLU:CB	2.28	0.62
1:H:147:ARG:HH22	1:H:330:ILE:CD1	2.12	0.62
1:E:72:GLU:HA	1:E:183:ARG:NH2	2.14	0.62
1:E:122:ILE:O	1:E:126:THR:HB	1.99	0.62
1:F:109:PRO:O	1:F:177:ARG:HD3	1.99	0.62
1:G:279:TYR:CD2	1:G:320:LEU:HD13	2.34	0.62
1:G:329:ILE:HD13	1:G:329:ILE:N	2.04	0.62
1:H:122:ILE:O	1:H:126:THR:HB	2.00	0.62
1:H:162:ASN:ND2	1:H:278:THR:HG22	2.12	0.62
1:H:315:LYS:HB2	1:H:315:LYS:NZ	2.13	0.62
1:D:105:LEU:HD22	1:D:105:LEU:H	1.65	0.62
1:H:136:ILE:HG23	1:H:139:VAL:HB	1.82	0.62
1:D:113:LYS:HG2	1:D:117:GLU:OE1	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:THR:HG22	1:D:205:GLU:CB	2.29	0.62
1:H:71:ILE:HG13	1:H:75:ILE:C	2.18	0.62
1:D:362:TYR:O	1:D:365:ALA:O	2.18	0.61
1:F:257:CYS:SG	1:F:258:PRO:HD3	2.40	0.61
1:G:238:LYS:HG2	1:G:254:ARG:HH12	1.60	0.61
1:D:110:LEU:HD11	1:D:175:ILE:HB	1.81	0.61
1:E:362:TYR:O	1:E:365:ALA:O	2.18	0.61
1:G:122:ILE:O	1:G:126:THR:HB	1.99	0.61
1:H:7:ALA:O	1:H:22:ALA:N	2.32	0.61
1:D:122:ILE:O	1:D:126:THR:HB	2.01	0.61
1:E:227:MET:HA	1:E:255:PHE:HZ	1.65	0.61
1:E:238:LYS:HG2	1:E:254:ARG:HH12	1.61	0.61
1:G:349:LEU:HB3	1:G:352:PHE:CE2	2.35	0.61
1:D:257:CYS:SG	1:D:258:PRO:HD3	2.40	0.61
1:E:274:ILE:HA	1:E:277:THR:OG1	2.00	0.61
1:F:255:PHE:O	1:F:258:PRO:HD2	1.99	0.61
1:G:209:VAL:O	1:G:212:ILE:HG12	2.00	0.61
1:G:257:CYS:SG	1:G:258:PRO:HD3	2.41	0.61
1:H:172:PRO:HA	1:H:175:ILE:HD11	1.81	0.61
1:H:289:ILE:HG23	1:H:289:ILE:O	2.00	0.61
1:E:91:TYR:O	1:E:92:ASN:CB	2.48	0.61
1:F:71:ILE:HG13	1:F:75:ILE:C	2.20	0.61
1:G:226:GLU:HA	1:G:229:THR:HG22	1.82	0.61
1:F:226:GLU:HA	1:F:229:THR:HG22	1.82	0.61
1:D:315:LYS:NZ	1:D:315:LYS:HB2	2.16	0.61
1:F:279:TYR:CD2	1:F:320:LEU:HD13	2.36	0.61
1:F:136:ILE:HG23	1:F:139:VAL:HB	1.83	0.61
1:H:279:TYR:CD2	1:H:320:LEU:HD13	2.35	0.61
1:E:221:LEU:HD12	1:E:221:LEU:N	2.16	0.60
1:F:52:SER:HB2	1:F:65:LEU:HD13	1.81	0.60
1:D:372:ARG:O	1:D:373:LYS:HB3	1.99	0.60
1:F:162:ASN:ND2	1:F:278:THR:HG22	2.14	0.60
1:F:261:LEU:O	1:F:274:ILE:HG12	2.00	0.60
1:E:51:ASP:HB3	1:E:53:TYR:CZ	2.36	0.60
1:G:359:LYS:O	1:G:360:GLN:HB3	2.02	0.60
1:D:274:ILE:HA	1:D:277:THR:OG1	2.01	0.60
1:E:240:TYR:CE1	1:E:241:GLU:O	2.55	0.60
1:G:97:ALA:HB3	1:G:100:GLU:OE2	2.02	0.60
1:G:113:LYS:HG2	1:G:117:GLU:OE1	2.01	0.60
1:G:273:GLY:O	1:G:277:THR:N	2.32	0.60
1:D:261:LEU:O	1:D:274:ILE:HG12	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ARG:HB3	1:F:204:ALA:CB	2.30	0.60
1:F:187:ASP:HA	1:F:190:MET:HE3	1.83	0.60
1:G:315:LYS:HB2	1:G:315:LYS:NZ	2.14	0.60
1:D:113:LYS:HE2	1:E:195:GLU:HG3	1.84	0.60
1:D:209:VAL:O	1:D:212:ILE:HG12	2.01	0.60
1:F:238:LYS:HZ2	1:F:254:ARG:HH22	1.48	0.60
1:F:289:ILE:O	1:F:289:ILE:HG23	2.02	0.60
1:F:315:LYS:HB2	1:F:315:LYS:NZ	2.16	0.60
1:H:52:SER:HB2	1:H:65:LEU:HD13	1.81	0.60
1:E:329:ILE:HD13	1:E:329:ILE:N	2.06	0.60
1:F:51:ASP:HB3	1:F:53:TYR:CZ	2.37	0.60
1:D:352:PHE:O	1:D:355:MET:HG2	2.02	0.60
1:E:226:GLU:HA	1:E:229:THR:HG22	1.83	0.60
1:E:372:ARG:O	1:E:373:LYS:HB3	2.02	0.60
1:G:109:PRO:CG	1:G:136:ILE:HG12	2.32	0.60
1:G:136:ILE:HG23	1:G:139:VAL:HB	1.83	0.60
1:H:7:ALA:O	1:H:22:ALA:HA	2.02	0.60
1:H:220:ALA:CB	1:H:226:GLU:HG3	2.32	0.60
1:E:238:LYS:HD3	1:E:239:SER:H	1.66	0.59
1:F:352:PHE:HZ	1:H:47:MET:HE1	1.66	0.59
1:E:62:ARG:HB3	1:E:204:ALA:CB	2.31	0.59
1:E:315:LYS:HB2	1:E:315:LYS:NZ	2.17	0.59
1:F:7:ALA:O	1:F:22:ALA:HA	2.02	0.59
1:D:349:LEU:HB3	1:D:352:PHE:CE2	2.36	0.59
1:E:7:ALA:O	1:E:22:ALA:HA	2.02	0.59
1:F:105:LEU:HD22	1:F:105:LEU:H	1.67	0.59
1:G:210:ARG:O	1:G:211:ASP:CB	2.50	0.59
1:G:289:ILE:HG23	1:G:289:ILE:O	2.01	0.59
1:D:267:ILE:O	1:D:267:ILE:HD13	2.02	0.59
1:E:257:CYS:SG	1:E:258:PRO:HD3	2.43	0.59
1:F:359:LYS:O	1:F:360:GLN:HB3	2.02	0.59
1:G:76:ILE:HG21	1:G:79:TRP:CE3	2.37	0.59
1:D:238:LYS:HD3	1:D:239:SER:H	1.67	0.59
1:D:51:ASP:HB3	1:D:53:TYR:CZ	2.36	0.59
1:D:173:HIS:CE1	1:E:268:GLY:HA3	2.37	0.59
1:D:210:ARG:O	1:D:211:ASP:CB	2.49	0.59
1:D:236:LEU:HD13	1:D:236:LEU:H	1.68	0.59
1:E:170:ALA:C	1:G:40:HIS:HE2	2.05	0.59
1:E:136:ILE:HG23	1:E:139:VAL:HB	1.84	0.59
1:E:272:ALA:HB1	1:E:277:THR:CG2	2.32	0.59
1:H:258:PRO:HG3	1:H:306:TYR:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:PRO:CB	1:E:127:PHE:HB3	2.28	0.59
1:E:209:VAL:O	1:E:212:ILE:HG12	2.03	0.59
1:G:98:PRO:CB	1:G:127:PHE:HB3	2.28	0.59
1:H:76:ILE:HG21	1:H:79:TRP:CE3	2.37	0.59
1:H:102:PRO:HB2	1:H:356:TRP:CZ3	2.38	0.59
1:H:187:ASP:HA	1:H:190:MET:HE3	1.85	0.59
1:H:238:LYS:HD3	1:H:239:SER:H	1.67	0.59
1:D:76:ILE:HG21	1:D:79:TRP:CE3	2.38	0.59
1:F:76:ILE:HG21	1:F:79:TRP:CE3	2.38	0.59
1:F:273:GLY:O	1:F:277:THR:N	2.27	0.59
1:H:36:GLY:O	1:H:65:LEU:HD11	2.03	0.59
1:H:226:GLU:HA	1:H:229:THR:HG22	1.84	0.59
1:D:352:PHE:HZ	1:F:47:MET:HE1	1.68	0.59
1:G:182:GLY:O	1:G:185:LEU:HB3	2.03	0.59
1:D:34:ILE:HG12	1:D:67:LEU:HD23	1.85	0.58
1:F:202:THR:HG22	1:F:205:GLU:CB	2.31	0.58
1:H:51:ASP:HB3	1:H:53:TYR:CZ	2.39	0.58
1:E:97:ALA:HB3	1:E:100:GLU:OE2	2.03	0.58
1:F:164:PRO:C	1:F:165:ILE:HD12	2.24	0.58
1:F:345:ILE:HG22	1:F:349:LEU:HD12	1.85	0.58
1:G:227:MET:HA	1:G:255:PHE:HZ	1.68	0.58
1:D:227:MET:HA	1:D:255:PHE:HZ	1.67	0.58
1:F:272:ALA:HB1	1:F:277:THR:CG2	2.34	0.58
1:F:182:GLY:O	1:F:185:LEU:HB3	2.03	0.58
1:G:62:ARG:HB3	1:G:204:ALA:CB	2.32	0.58
1:E:183:ARG:O	1:E:186:THR:HB	2.04	0.58
1:E:210:ARG:O	1:E:211:ASP:CB	2.51	0.58
1:F:109:PRO:CG	1:F:136:ILE:HG12	2.31	0.58
1:F:123:MET:HA	1:F:127:PHE:HD2	1.69	0.58
1:G:51:ASP:HB3	1:G:53:TYR:CZ	2.37	0.58
1:H:355:MET:HE2	1:H:356:TRP:HE1	1.69	0.58
1:H:240:TYR:CE1	1:H:241:GLU:O	2.57	0.58
1:G:238:LYS:HD3	1:G:239:SER:H	1.68	0.58
1:H:209:VAL:O	1:H:212:ILE:HG12	2.02	0.58
1:H:221:LEU:HD12	1:H:221:LEU:N	2.19	0.58
1:H:221:LEU:HD23	1:H:315:LYS:HD3	1.85	0.58
1:H:372:ARG:O	1:H:373:LYS:HB3	2.03	0.58
1:D:164:PRO:C	1:D:165:ILE:HD12	2.24	0.58
1:D:170:ALA:C	1:F:40:HIS:HE2	2.07	0.58
1:H:123:MET:HA	1:H:127:PHE:HD2	1.69	0.58
1:H:183:ARG:O	1:H:186:THR:HB	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:MET:HA	1:H:255:PHE:HZ	1.69	0.58
1:D:7:ALA:O	1:D:22:ALA:HA	2.04	0.58
1:H:258:PRO:O	1:H:261:LEU:HD12	2.03	0.58
1:H:345:ILE:HG22	1:H:349:LEU:HD12	1.85	0.58
1:D:153:LEU:HA	1:D:161:HIS:O	2.03	0.58
1:D:154:ASP:HA	1:D:300:SER:O	2.02	0.58
1:F:220:ALA:CB	1:F:226:GLU:HG3	2.34	0.58
1:G:36:GLY:O	1:G:65:LEU:HD11	2.04	0.58
1:D:255:PHE:O	1:D:258:PRO:HD2	2.03	0.57
1:D:305:MET:O	1:D:306:TYR:C	2.42	0.57
1:D:355:MET:HE2	1:D:356:TRP:HE1	1.68	0.57
1:G:355:MET:HE2	1:G:356:TRP:HE1	1.68	0.57
1:D:284:LYS:HE2	1:D:284:LYS:HA	1.86	0.57
1:E:79:TRP:CZ2	1:E:118:LYS:HB3	2.39	0.57
1:F:170:ALA:C	1:H:40:HIS:HE2	2.08	0.57
1:G:345:ILE:HG22	1:G:349:LEU:HD12	1.85	0.57
1:D:163:VAL:HG13	1:D:165:ILE:CD1	2.34	0.57
1:E:105:LEU:H	1:E:105:LEU:HD22	1.67	0.57
1:E:172:PRO:HA	1:E:175:ILE:HD11	1.85	0.57
1:G:221:LEU:HD12	1:G:221:LEU:N	2.19	0.57
1:F:136:ILE:HD12	1:F:139:VAL:H	1.70	0.57
1:F:185:LEU:HD13	1:F:185:LEU:O	2.05	0.57
1:F:210:ARG:O	1:F:211:ASP:HB3	2.05	0.57
1:F:258:PRO:HG3	1:F:306:TYR:CE2	2.39	0.57
1:F:355:MET:HE2	1:F:356:TRP:HE1	1.70	0.57
1:F:372:ARG:O	1:F:373:LYS:HB3	2.03	0.57
1:H:250:ILE:O	1:H:251:GLY:O	2.22	0.57
1:E:5:THR:OG1	1:E:102:PRO:HD2	2.04	0.57
1:E:20:GLY:HA3	1:E:340:TRP:HZ2	1.68	0.57
1:E:258:PRO:O	1:E:261:LEU:HD12	2.05	0.57
1:G:372:ARG:O	1:G:373:LYS:HB3	2.04	0.57
1:H:105:LEU:H	1:H:105:LEU:HD22	1.68	0.57
1:H:242:LEU:C	1:H:242:LEU:HD12	2.25	0.57
1:H:284:LYS:HE2	1:H:284:LYS:HA	1.87	0.57
1:D:258:PRO:O	1:D:261:LEU:HD12	2.05	0.57
1:E:329:ILE:H	1:E:329:ILE:CD1	2.04	0.57
1:F:36:GLY:O	1:F:65:LEU:HD11	2.04	0.57
1:G:7:ALA:O	1:G:22:ALA:HA	2.04	0.57
1:H:225:ASN:O	1:H:229:THR:HG22	2.05	0.57
1:F:34:ILE:HG12	1:F:67:LEU:HD23	1.87	0.57
1:D:172:PRO:HA	1:D:175:ILE:HD11	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:LEU:HD12	1:F:221:LEU:N	2.19	0.57
1:F:325:MET:SD	1:H:244:ASP:CG	2.82	0.57
1:G:258:PRO:HG3	1:G:306:TYR:CE2	2.36	0.57
1:D:20:GLY:HA3	1:D:340:TRP:HZ2	1.70	0.57
1:D:79:TRP:CZ2	1:D:118:LYS:HB3	2.39	0.57
1:D:97:ALA:HB3	1:D:100:GLU:OE2	2.04	0.57
1:D:98:PRO:CB	1:D:127:PHE:HB3	2.29	0.57
1:F:20:GLY:HA3	1:F:340:TRP:HZ2	1.70	0.57
1:G:136:ILE:HD12	1:G:139:VAL:H	1.69	0.57
1:D:9:VAL:HG21	1:D:344:SER:HA	1.87	0.57
1:F:9:VAL:HG21	1:F:344:SER:HA	1.87	0.57
1:F:345:ILE:O	1:F:349:LEU:HB2	2.05	0.57
1:G:162:ASN:ND2	1:G:278:THR:HG22	2.14	0.57
1:G:258:PRO:O	1:G:261:LEU:HD12	2.05	0.57
1:D:62:ARG:HB3	1:D:204:ALA:CB	2.34	0.56
1:D:78:ASN:HB3	1:D:81:ASP:CG	2.25	0.56
1:E:136:ILE:HD12	1:E:139:VAL:H	1.70	0.56
1:E:163:VAL:HG13	1:E:165:ILE:CD1	2.35	0.56
1:F:43:VAL:HG13	1:F:44:MET:N	2.20	0.56
1:H:97:ALA:HB3	1:H:100:GLU:OE2	2.05	0.56
1:D:162:ASN:ND2	1:D:278:THR:HG22	2.18	0.56
1:E:201:VAL:H	1:E:205:GLU:CD	2.06	0.56
1:F:329:ILE:H	1:F:329:ILE:CD1	2.07	0.56
1:G:34:ILE:HG12	1:G:67:LEU:HD23	1.86	0.56
1:D:109:PRO:HD2	1:D:161:HIS:CE1	2.40	0.56
1:D:226:GLU:HA	1:D:229:THR:CG2	2.35	0.56
1:D:258:PRO:HG3	1:D:306:TYR:CE2	2.39	0.56
1:D:273:GLY:O	1:D:277:THR:N	2.32	0.56
1:E:185:LEU:C	1:E:185:LEU:HD13	2.26	0.56
1:E:186:THR:O	1:E:189:LEU:HB2	2.05	0.56
1:E:314:GLN:HE22	1:E:327:ILE:HG12	1.70	0.56
1:E:345:ILE:HG22	1:E:349:LEU:HD12	1.87	0.56
1:F:78:ASN:HB3	1:F:81:ASP:CG	2.25	0.56
1:F:225:ASN:O	1:F:229:THR:HG22	2.06	0.56
1:F:238:LYS:HD3	1:F:239:SER:H	1.69	0.56
1:G:102:PRO:HB2	1:G:356:TRP:CZ3	2.40	0.56
1:G:105:LEU:HD22	1:G:105:LEU:H	1.69	0.56
1:G:123:MET:HA	1:G:127:PHE:HD2	1.70	0.56
1:G:183:ARG:O	1:G:186:THR:HB	2.05	0.56
1:G:220:ALA:CB	1:G:226:GLU:HG3	2.33	0.56
1:G:250:ILE:O	1:G:251:GLY:O	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:CYS:O	1:G:375:PHE:HB3	2.04	0.56
1:H:272:ALA:HB1	1:H:277:THR:CG2	2.35	0.56
1:D:201:VAL:H	1:D:205:GLU:CD	2.07	0.56
1:D:359:LYS:O	1:D:360:GLN:HB3	2.05	0.56
1:E:202:THR:HG23	1:E:203:THR:N	2.20	0.56
1:E:349:LEU:HB3	1:E:352:PHE:CD2	2.41	0.56
1:F:97:ALA:HB3	1:F:100:GLU:OE2	2.05	0.56
1:G:153:LEU:HA	1:G:161:HIS:O	2.05	0.56
1:G:164:PRO:C	1:G:165:ILE:HD12	2.25	0.56
1:G:305:MET:O	1:G:306:TYR:C	2.42	0.56
1:H:34:ILE:HG12	1:H:67:LEU:HD23	1.87	0.56
1:D:289:ILE:HG23	1:D:289:ILE:O	2.06	0.56
1:E:20:GLY:HA3	1:E:340:TRP:CZ2	2.40	0.56
1:E:162:ASN:ND2	1:E:278:THR:HG22	2.15	0.56
1:E:164:PRO:C	1:E:165:ILE:HD12	2.24	0.56
1:E:220:ALA:CB	1:E:226:GLU:HG3	2.33	0.56
1:E:227:MET:HG2	1:E:255:PHE:CE1	2.41	0.56
1:E:242:LEU:C	1:E:242:LEU:HD12	2.26	0.56
1:G:259:GLU:CB	1:G:263:GLN:HE22	1.99	0.56
1:H:5:THR:OG1	1:H:102:PRO:HD2	2.05	0.56
1:H:43:VAL:HG13	1:H:44:MET:N	2.20	0.56
1:H:359:LYS:O	1:H:360:GLN:HB3	2.04	0.56
1:D:136:ILE:HD12	1:D:139:VAL:H	1.71	0.56
1:D:221:LEU:HD12	1:D:221:LEU:N	2.20	0.56
1:D:314:GLN:HE22	1:D:327:ILE:HG12	1.70	0.56
1:E:34:ILE:HG12	1:E:67:LEU:HD23	1.86	0.56
1:G:5:THR:OG1	1:G:102:PRO:HD2	2.05	0.56
1:H:257:CYS:SG	1:H:258:PRO:CD	2.94	0.56
1:D:102:PRO:HB2	1:D:356:TRP:CZ3	2.41	0.56
1:D:227:MET:HG2	1:D:255:PHE:CE1	2.40	0.56
1:D:325:MET:SD	1:F:244:ASP:CG	2.84	0.56
1:D:345:ILE:O	1:D:349:LEU:HB2	2.06	0.56
1:E:109:PRO:CG	1:E:136:ILE:HG12	2.32	0.56
1:F:5:THR:OG1	1:F:102:PRO:HD2	2.05	0.56
1:F:216:LEU:HD13	1:F:250:ILE:CG1	2.36	0.56
1:F:222:ASP:O	1:F:224:GLU:N	2.39	0.56
1:H:163:VAL:HG13	1:H:165:ILE:CD1	2.35	0.56
1:H:164:PRO:C	1:H:165:ILE:HD12	2.26	0.56
1:H:314:GLN:HE22	1:H:327:ILE:HG12	1.70	0.56
1:D:5:THR:OG1	1:D:102:PRO:HD2	2.05	0.56
1:D:183:ARG:O	1:D:186:THR:HB	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:THR:O	1:D:189:LEU:HB2	2.05	0.56
1:E:284:LYS:HE2	1:E:284:LYS:HA	1.88	0.56
1:F:201:VAL:H	1:F:205:GLU:CD	2.08	0.56
1:F:314:GLN:HE22	1:F:327:ILE:HG12	1.70	0.56
1:G:79:TRP:CZ2	1:G:118:LYS:HB3	2.41	0.56
1:G:314:GLN:HE22	1:G:327:ILE:HG12	1.70	0.56
1:D:20:GLY:HA3	1:D:340:TRP:CZ2	2.41	0.56
1:E:355:MET:HE2	1:E:356:TRP:HE1	1.69	0.56
1:F:183:ARG:O	1:F:186:THR:HB	2.06	0.56
1:F:263:GLN:C	1:F:265:SER:H	2.09	0.56
1:G:238:LYS:HZ2	1:G:254:ARG:HH22	1.54	0.56
1:G:339:VAL:HG23	1:G:340:TRP:N	2.21	0.56
1:H:123:MET:O	1:H:127:PHE:HB2	2.06	0.56
1:H:253:GLU:CD	1:H:253:GLU:H	2.09	0.56
1:H:357:ILE:CD1	1:H:370:VAL:HG23	2.36	0.56
1:D:36:GLY:O	1:D:65:LEU:HD11	2.06	0.56
1:E:173:HIS:CE1	1:F:268:GLY:HA3	2.41	0.56
1:E:222:ASP:O	1:E:224:GLU:N	2.38	0.56
1:F:102:PRO:HB2	1:F:356:TRP:CZ3	2.41	0.56
1:F:305:MET:O	1:F:306:TYR:C	2.44	0.56
1:G:317:ILE:HD13	1:G:317:ILE:N	2.19	0.56
1:H:202:THR:HG23	1:H:203:THR:N	2.21	0.56
1:D:202:THR:HG23	1:D:203:THR:N	2.21	0.55
1:D:220:ALA:CB	1:D:226:GLU:HG3	2.36	0.55
1:G:122:ILE:HG22	1:G:123:MET:HE2	1.88	0.55
1:G:222:ASP:O	1:G:224:GLU:N	2.38	0.55
1:H:136:ILE:HD12	1:H:139:VAL:H	1.70	0.55
1:H:317:ILE:HD13	1:H:317:ILE:N	2.22	0.55
1:D:62:ARG:HE	1:D:208:ILE:HD11	1.71	0.55
1:D:216:LEU:HD13	1:D:250:ILE:CG1	2.36	0.55
1:D:253:GLU:H	1:D:253:GLU:CD	2.10	0.55
1:E:76:ILE:N	1:E:115:ASN:HD21	1.96	0.55
1:E:76:ILE:HG21	1:E:79:TRP:CE3	2.41	0.55
1:E:339:VAL:HG23	1:E:340:TRP:N	2.21	0.55
1:F:320:LEU:HD12	1:F:321:ALA:H	1.70	0.55
1:G:272:ALA:HB1	1:G:277:THR:CG2	2.35	0.55
1:G:345:ILE:O	1:G:349:LEU:HB2	2.06	0.55
1:E:221:LEU:HD23	1:E:315:LYS:HD3	1.88	0.55
1:E:253:GLU:CD	1:E:253:GLU:H	2.10	0.55
1:F:153:LEU:HA	1:F:161:HIS:O	2.06	0.55
1:G:67:LEU:HD12	1:G:67:LEU:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:LEU:CB	1:H:177:ARG:HG3	2.33	0.55
1:D:272:ALA:HB1	1:D:277:THR:CG2	2.36	0.55
1:E:238:LYS:HZ3	1:E:254:ARG:HH22	1.54	0.55
1:F:210:ARG:O	1:F:211:ASP:CB	2.54	0.55
1:G:173:HIS:CE1	1:H:268:GLY:HA3	2.41	0.55
1:G:221:LEU:HD23	1:G:315:LYS:HD3	1.89	0.55
1:H:78:ASN:HB3	1:H:81:ASP:CG	2.27	0.55
1:D:286:ASP:HB3	1:D:289:ILE:CG2	2.36	0.55
1:E:78:ASN:HB3	1:E:81:ASP:CG	2.26	0.55
1:E:286:ASP:HB3	1:E:289:ILE:CG2	2.36	0.55
1:F:20:GLY:HA3	1:F:340:TRP:CZ2	2.41	0.55
1:F:227:MET:HG2	1:F:255:PHE:CE1	2.42	0.55
1:H:210:ARG:O	1:H:211:ASP:HB3	2.05	0.55
1:H:345:ILE:O	1:H:349:LEU:HB2	2.05	0.55
1:D:339:VAL:HG23	1:D:340:TRP:N	2.22	0.55
1:F:91:TYR:O	1:F:92:ASN:HB3	2.07	0.55
1:F:350:SER:C	1:F:352:PHE:N	2.57	0.55
1:G:109:PRO:HD2	1:G:161:HIS:CE1	2.40	0.55
1:H:227:MET:HG2	1:H:255:PHE:CE1	2.42	0.55
1:E:219:VAL:HG23	1:E:220:ALA:N	2.22	0.55
1:E:352:PHE:HZ	1:G:47:MET:HE1	1.71	0.55
1:F:79:TRP:CZ2	1:F:118:LYS:HB3	2.42	0.55
1:F:163:VAL:HG13	1:F:165:ILE:CD1	2.36	0.55
1:G:241:GLU:OE1	1:G:247:VAL:HG22	2.07	0.55
1:G:242:LEU:C	1:G:242:LEU:HD12	2.27	0.55
1:E:102:PRO:HB2	1:E:356:TRP:CZ3	2.42	0.55
1:F:317:ILE:HD13	1:F:317:ILE:N	2.22	0.55
1:G:76:ILE:N	1:G:115:ASN:HD21	1.96	0.55
1:G:98:PRO:HG3	1:G:127:PHE:CD1	2.41	0.55
1:G:123:MET:O	1:G:127:PHE:HB2	2.07	0.55
1:H:267:ILE:O	1:H:267:ILE:HD13	2.06	0.55
1:D:123:MET:HA	1:D:127:PHE:HD2	1.72	0.55
1:D:263:GLN:C	1:D:265:SER:H	2.10	0.55
1:E:305:MET:O	1:E:306:TYR:C	2.44	0.55
1:G:263:GLN:O	1:G:263:GLN:HG2	2.07	0.55
1:D:109:PRO:CG	1:D:136:ILE:HG12	2.34	0.55
1:E:123:MET:O	1:E:127:PHE:HB2	2.07	0.55
1:F:257:CYS:SG	1:F:258:PRO:CD	2.95	0.55
1:F:332:PRO:HB2	1:F:334:GLU:OE1	2.07	0.55
1:G:20:GLY:HA3	1:G:340:TRP:HZ2	1.72	0.55
1:G:235:SER:HB2	1:G:236:LEU:HD13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:PRO:HB2	1:G:334:GLU:OE1	2.07	0.55
1:H:182:GLY:O	1:H:185:LEU:HB3	2.06	0.55
1:H:241:GLU:OE1	1:H:247:VAL:HG22	2.07	0.55
1:D:181:ALA:HB3	1:D:184:ASP:OD1	2.06	0.54
1:D:185:LEU:HD13	1:D:185:LEU:C	2.27	0.54
1:D:345:ILE:HG22	1:D:349:LEU:HD12	1.89	0.54
1:D:358:THR:H	1:D:361:GLU:CD	2.10	0.54
1:E:216:LEU:HD13	1:E:250:ILE:CG1	2.35	0.54
1:F:221:LEU:HD23	1:F:315:LYS:HD3	1.88	0.54
1:D:20:GLY:CA	1:D:340:TRP:HZ2	2.21	0.54
1:E:225:ASN:O	1:E:229:THR:HG22	2.08	0.54
1:E:235:SER:HB2	1:E:236:LEU:HD13	1.89	0.54
1:E:325:MET:SD	1:G:244:ASP:CG	2.86	0.54
1:F:75:ILE:HA	1:F:111:ASN:HD21	1.72	0.54
1:G:112:PRO:HA	1:H:194:THR:O	2.07	0.54
1:G:163:VAL:HG13	1:G:165:ILE:CD1	2.36	0.54
1:H:98:PRO:CB	1:H:127:PHE:HB3	2.31	0.54
1:E:241:GLU:OE1	1:E:247:VAL:HG22	2.07	0.54
1:E:304:THR:HG22	1:E:335:ARG:HD3	1.88	0.54
1:F:76:ILE:N	1:F:115:ASN:HD21	1.93	0.54
1:G:201:VAL:H	1:G:205:GLU:CD	2.10	0.54
1:G:277:THR:HA	1:G:280:ASN:ND2	2.23	0.54
1:H:221:LEU:CB	1:H:315:LYS:HE2	2.38	0.54
1:F:186:THR:O	1:F:189:LEU:HB2	2.07	0.54
1:G:286:ASP:HB3	1:G:289:ILE:CG2	2.37	0.54
1:H:201:VAL:H	1:H:205:GLU:CD	2.10	0.54
1:H:258:PRO:HA	1:H:261:LEU:HD12	1.88	0.54
1:D:122:ILE:HG22	1:D:123:MET:HE2	1.90	0.54
1:D:369:ILE:HG13	1:D:372:ARG:NH2	2.23	0.54
1:F:123:MET:O	1:F:127:PHE:HB2	2.08	0.54
1:H:136:ILE:HD13	1:H:138:ALA:N	2.22	0.54
1:H:339:VAL:HG23	1:H:340:TRP:N	2.21	0.54
1:D:317:ILE:HD13	1:D:317:ILE:N	2.23	0.54
1:D:320:LEU:HD12	1:D:321:ALA:H	1.73	0.54
1:F:189:LEU:CD1	1:F:213:LYS:HB3	2.37	0.54
1:F:299:MET:HB3	1:F:304:THR:HG23	1.89	0.54
1:G:225:ASN:O	1:G:229:THR:HG22	2.08	0.54
1:G:253:GLU:H	1:G:253:GLU:CD	2.10	0.54
1:H:108:ALA:HA	1:H:137:GLN:HG2	1.89	0.54
1:E:185:LEU:HD13	1:E:185:LEU:O	2.07	0.54
1:E:369:ILE:HG13	1:E:372:ARG:NH2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:PRO:HD2	1:F:161:HIS:CE1	2.43	0.54
1:H:110:LEU:HB2	1:H:177:ARG:CG	2.34	0.54
1:D:257:CYS:SG	1:D:258:PRO:CD	2.96	0.54
1:F:250:ILE:O	1:F:251:GLY:O	2.25	0.54
1:F:258:PRO:HA	1:F:261:LEU:HD12	1.90	0.54
1:F:339:VAL:HG23	1:F:340:TRP:N	2.23	0.54
1:G:9:VAL:HG21	1:G:344:SER:HA	1.90	0.54
1:G:154:ASP:HA	1:G:300:SER:O	2.07	0.54
1:G:216:LEU:HD13	1:G:250:ILE:CG1	2.36	0.54
1:D:332:PRO:HB2	1:D:334:GLU:OE1	2.08	0.54
1:E:123:MET:HA	1:E:127:PHE:HD2	1.72	0.54
1:F:122:ILE:HG22	1:F:123:MET:HE2	1.90	0.54
1:F:202:THR:HG23	1:F:203:THR:N	2.23	0.54
1:G:79:TRP:HA	1:G:79:TRP:HE3	1.72	0.54
1:H:109:PRO:HD2	1:H:161:HIS:CE1	2.42	0.54
1:D:350:SER:C	1:D:352:PHE:N	2.60	0.54
1:G:257:CYS:SG	1:G:258:PRO:CD	2.96	0.54
1:D:139:VAL:HG21	1:F:43:VAL:HG21	1.90	0.53
1:D:221:LEU:HD23	1:D:315:LYS:HD3	1.90	0.53
1:E:109:PRO:HD2	1:E:161:HIS:CE1	2.41	0.53
1:G:91:TYR:O	1:G:92:ASN:HB3	2.06	0.53
1:H:163:VAL:HG22	1:H:165:ILE:HD11	1.90	0.53
1:H:305:MET:O	1:H:306:TYR:C	2.45	0.53
1:H:332:PRO:HB2	1:H:334:GLU:OE1	2.08	0.53
1:D:263:GLN:O	1:D:263:GLN:HG2	2.07	0.53
1:E:62:ARG:HE	1:E:208:ILE:HD11	1.73	0.53
1:E:289:ILE:HG23	1:E:289:ILE:O	2.06	0.53
1:F:98:PRO:HG3	1:F:127:PHE:CD1	2.44	0.53
1:F:173:HIS:CE1	1:G:268:GLY:HA3	2.42	0.53
1:G:202:THR:HG23	1:G:203:THR:N	2.22	0.53
1:D:250:ILE:O	1:D:251:GLY:O	2.27	0.53
1:E:67:LEU:N	1:E:67:LEU:HD12	2.24	0.53
1:F:258:PRO:O	1:F:261:LEU:HD12	2.08	0.53
1:H:98:PRO:HG3	1:H:127:PHE:CD1	2.44	0.53
1:E:277:THR:HA	1:E:280:ASN:ND2	2.24	0.53
1:E:358:THR:H	1:E:361:GLU:CD	2.10	0.53
1:F:320:LEU:HD12	1:F:321:ALA:N	2.24	0.53
1:G:181:ALA:HB3	1:G:184:ASP:OD1	2.09	0.53
1:G:189:LEU:CD1	1:G:213:LYS:HB3	2.36	0.53
1:H:185:LEU:C	1:H:185:LEU:HD13	2.28	0.53
1:H:235:SER:HB2	1:H:236:LEU:HD13	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:MET:HB3	1:H:304:THR:HG23	1.89	0.53
1:D:277:THR:HA	1:D:280:ASN:ND2	2.23	0.53
1:D:304:THR:HG22	1:D:335:ARG:HD3	1.90	0.53
1:E:7:ALA:O	1:E:22:ALA:CA	2.57	0.53
1:E:263:GLN:C	1:E:265:SER:H	2.12	0.53
1:F:112:PRO:HA	1:G:194:THR:O	2.08	0.53
1:F:277:THR:HA	1:F:280:ASN:ND2	2.23	0.53
1:G:78:ASN:HB3	1:G:81:ASP:CG	2.27	0.53
1:G:255:PHE:O	1:G:258:PRO:HD2	2.08	0.53
1:G:284:LYS:HE2	1:G:284:LYS:HA	1.90	0.53
1:H:349:LEU:HB3	1:H:352:PHE:CD2	2.43	0.53
1:E:20:GLY:CA	1:E:340:TRP:HZ2	2.21	0.53
1:E:108:ALA:HA	1:E:137:GLN:HG2	1.91	0.53
1:E:317:ILE:N	1:E:317:ILE:HD13	2.23	0.53
1:F:59:GLN:HE21	1:F:62:ARG:HH21	1.57	0.53
1:H:238:LYS:HZ3	1:H:254:ARG:HH22	1.54	0.53
1:D:123:MET:O	1:D:127:PHE:HB2	2.08	0.53
1:D:187:ASP:HA	1:D:190:MET:HE3	1.91	0.53
1:F:7:ALA:O	1:F:22:ALA:CA	2.57	0.53
1:F:20:GLY:CA	1:F:340:TRP:HZ2	2.22	0.53
1:F:185:LEU:HD13	1:F:185:LEU:C	2.29	0.53
1:G:108:ALA:HA	1:G:137:GLN:HG2	1.91	0.53
1:G:358:THR:H	1:G:361:GLU:CD	2.12	0.53
1:G:20:GLY:HA3	1:G:340:TRP:CZ2	2.44	0.53
1:G:240:TYR:CE1	1:G:241:GLU:O	2.62	0.53
1:G:263:GLN:C	1:G:265:SER:H	2.12	0.53
1:G:299:MET:HB3	1:G:304:THR:HG23	1.91	0.53
1:G:336:LYS:HD2	1:G:336:LYS:O	2.09	0.53
1:H:9:VAL:HG21	1:H:344:SER:HA	1.91	0.53
1:H:263:GLN:C	1:H:265:SER:H	2.12	0.53
1:D:66:THR:HG23	1:D:203:THR:CG2	2.29	0.53
1:E:202:THR:CG2	1:E:205:GLU:HB2	2.34	0.53
1:E:229:THR:HG23	1:E:230:ALA:N	2.24	0.53
1:F:44:MET:CE	1:F:45:VAL:H	2.22	0.53
1:F:241:GLU:OE1	1:F:247:VAL:HG22	2.09	0.53
1:F:253:GLU:CD	1:F:253:GLU:H	2.12	0.53
1:G:369:ILE:HG13	1:G:372:ARG:NH2	2.24	0.53
1:H:79:TRP:HA	1:H:79:TRP:HE3	1.74	0.53
1:H:138:ALA:HB1	1:H:163:VAL:CG1	2.39	0.53
1:D:166:TYR:CD2	1:F:64:ILE:HG21	2.44	0.53
1:D:238:LYS:HZ2	1:D:254:ARG:NH2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:PRO:HG3	1:E:306:TYR:CE2	2.40	0.53
1:H:122:ILE:HG22	1:H:123:MET:HE2	1.90	0.53
1:D:76:ILE:N	1:D:115:ASN:HD21	1.95	0.52
1:D:169:TYR:HA	1:F:42:GLY:CA	2.36	0.52
1:E:99:GLU:CG	1:E:128:ASN:HB2	2.39	0.52
1:E:320:LEU:HD12	1:E:321:ALA:H	1.74	0.52
1:H:185:LEU:HD13	1:H:185:LEU:O	2.09	0.52
1:D:98:PRO:HG3	1:D:127:PHE:CD1	2.45	0.52
1:D:242:LEU:C	1:D:242:LEU:HD12	2.30	0.52
1:E:139:VAL:HG21	1:G:43:VAL:HG21	1.90	0.52
1:G:75:ILE:HA	1:G:111:ASN:HD21	1.74	0.52
1:D:79:TRP:HA	1:D:79:TRP:HE3	1.73	0.52
1:D:108:ALA:HA	1:D:137:GLN:HG2	1.92	0.52
1:E:139:VAL:HG22	1:G:43:VAL:HG11	1.91	0.52
1:E:299:MET:HB3	1:E:304:THR:HG23	1.90	0.52
1:H:44:MET:HE2	1:H:47:MET:HG2	1.92	0.52
1:H:44:MET:HE3	1:H:45:VAL:H	1.74	0.52
1:H:222:ASP:O	1:H:224:GLU:N	2.43	0.52
1:D:202:THR:CG2	1:D:205:GLU:HB2	2.36	0.52
1:D:258:PRO:HA	1:D:261:LEU:HD12	1.90	0.52
1:D:302:GLY:C	1:D:304:THR:N	2.63	0.52
1:E:112:PRO:HA	1:F:194:THR:O	2.09	0.52
1:G:43:VAL:HG13	1:G:44:MET:N	2.24	0.52
1:F:235:SER:HB2	1:F:236:LEU:HD13	1.90	0.52
1:F:284:LYS:HA	1:F:284:LYS:HE2	1.92	0.52
1:H:216:LEU:HD13	1:H:250:ILE:CG1	2.35	0.52
1:H:229:THR:HG23	1:H:230:ALA:N	2.24	0.52
1:D:163:VAL:HG22	1:D:165:ILE:HD11	1.91	0.52
1:D:235:SER:HB2	1:D:236:LEU:HD13	1.90	0.52
1:D:327:ILE:HD13	1:D:327:ILE:N	2.24	0.52
1:E:272:ALA:HB1	1:E:277:THR:HG21	1.91	0.52
1:F:34:ILE:C	1:F:34:ILE:HD12	2.30	0.52
1:F:349:LEU:HB3	1:F:352:PHE:CD2	2.43	0.52
1:F:355:MET:O	1:F:373:LYS:HE3	2.10	0.52
1:G:34:ILE:O	1:G:35:VAL:HG13	2.10	0.52
1:H:67:LEU:N	1:H:67:LEU:HD12	2.24	0.52
1:H:238:LYS:HZ2	1:H:254:ARG:HH22	1.58	0.52
1:H:350:SER:C	1:H:352:PHE:N	2.60	0.52
1:E:198:TYR:HB3	1:E:200:PHE:HE1	1.74	0.52
1:F:136:ILE:HD13	1:F:138:ALA:N	2.24	0.52
1:F:267:ILE:O	1:F:267:ILE:HD13	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:LEU:CB	1:G:177:ARG:HG3	2.37	0.52
1:G:304:THR:HG22	1:G:335:ARG:HD3	1.91	0.52
1:H:20:GLY:HA3	1:H:340:TRP:HZ2	1.75	0.52
1:H:340:TRP:CE3	1:H:341:ILE:HD13	2.41	0.52
1:H:358:THR:H	1:H:361:GLU:CD	2.13	0.52
1:D:153:LEU:HD13	1:D:313:MET:HE1	1.92	0.52
1:E:59:GLN:HE21	1:E:62:ARG:HH21	1.56	0.52
1:E:165:ILE:HG13	1:E:170:ALA:HB1	1.91	0.52
1:E:332:PRO:HB2	1:E:334:GLU:OE1	2.10	0.52
1:F:219:VAL:HG23	1:F:220:ALA:N	2.24	0.52
1:F:273:GLY:N	1:F:277:THR:HG23	2.19	0.52
1:G:202:THR:CG2	1:G:205:GLU:HB2	2.35	0.52
1:H:263:GLN:HG2	1:H:263:GLN:O	2.10	0.52
1:D:59:GLN:HE21	1:D:62:ARG:HH21	1.57	0.52
1:D:99:GLU:CG	1:D:128:ASN:HB2	2.40	0.52
1:E:9:VAL:HG21	1:E:344:SER:HA	1.92	0.52
1:E:98:PRO:HG3	1:E:127:PHE:CD1	2.45	0.52
1:E:226:GLU:HA	1:E:229:THR:CG2	2.40	0.52
1:E:350:SER:C	1:E:352:PHE:N	2.63	0.52
1:F:226:GLU:HA	1:F:229:THR:CG2	2.39	0.52
1:G:121:GLN:O	1:G:125:GLU:HG2	2.09	0.52
1:G:227:MET:HG2	1:G:255:PHE:CE1	2.45	0.52
1:G:355:MET:O	1:G:373:LYS:HE3	2.10	0.52
1:H:210:ARG:O	1:H:211:ASP:CB	2.57	0.52
1:H:304:THR:HG22	1:H:335:ARG:HD3	1.91	0.52
1:D:99:GLU:O	1:D:130:PRO:HB3	2.10	0.52
1:D:189:LEU:CD1	1:D:213:LYS:HB3	2.39	0.52
1:E:257:CYS:SG	1:E:258:PRO:CD	2.98	0.52
1:E:263:GLN:HG2	1:E:263:GLN:O	2.10	0.52
1:E:336:LYS:HD2	1:E:336:LYS:O	2.10	0.52
1:F:198:TYR:HB3	1:F:200:PHE:HE1	1.75	0.52
1:F:272:ALA:HB1	1:F:277:THR:HG21	1.92	0.52
1:G:187:ASP:HA	1:G:190:MET:HE3	1.92	0.52
1:G:357:ILE:CD1	1:G:370:VAL:HG23	2.40	0.52
1:G:370:VAL:O	1:G:374:CYS:SG	2.68	0.52
1:H:102:PRO:HB2	1:H:356:TRP:HZ3	1.73	0.52
1:D:219:VAL:O	1:D:220:ALA:HB3	2.09	0.51
1:D:229:THR:HG23	1:D:230:ALA:N	2.25	0.51
1:E:359:LYS:O	1:E:360:GLN:HB3	2.09	0.51
1:F:67:LEU:HD12	1:F:67:LEU:N	2.24	0.51
1:F:336:LYS:HD2	1:F:336:LYS:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:GLY:C	1:G:304:THR:N	2.63	0.51
1:H:273:GLY:H	1:H:277:THR:CG2	2.20	0.51
1:E:304:THR:CG2	1:E:335:ARG:HD3	2.39	0.51
1:F:166:TYR:CD2	1:H:64:ILE:HG21	2.45	0.51
1:F:358:THR:H	1:F:361:GLU:CD	2.12	0.51
1:G:20:GLY:CA	1:G:340:TRP:HZ2	2.22	0.51
1:G:219:VAL:O	1:G:220:ALA:HB3	2.09	0.51
1:H:273:GLY:N	1:H:277:THR:HG23	2.20	0.51
1:D:75:ILE:HA	1:D:111:ASN:HD21	1.74	0.51
1:D:136:ILE:HD12	1:D:139:VAL:CG2	2.35	0.51
1:D:185:LEU:HD13	1:D:185:LEU:O	2.10	0.51
1:E:79:TRP:HA	1:E:79:TRP:HE3	1.74	0.51
1:E:189:LEU:CD1	1:E:213:LYS:HB3	2.38	0.51
1:F:79:TRP:HA	1:F:79:TRP:HE3	1.75	0.51
1:G:136:ILE:HD13	1:G:138:ALA:N	2.26	0.51
1:G:229:THR:HG23	1:G:230:ALA:N	2.25	0.51
1:H:153:LEU:HD13	1:H:313:MET:HE1	1.92	0.51
1:H:163:VAL:HG22	1:H:165:ILE:CD1	2.40	0.51
1:H:189:LEU:CD1	1:H:213:LYS:HB3	2.38	0.51
1:H:286:ASP:HB3	1:H:289:ILE:CG2	2.38	0.51
1:E:36:GLY:O	1:E:65:LEU:HD11	2.10	0.51
1:E:267:ILE:O	1:E:267:ILE:HD13	2.10	0.51
1:E:345:ILE:O	1:E:349:LEU:HB2	2.10	0.51
1:G:226:GLU:HA	1:G:229:THR:CG2	2.41	0.51
1:H:59:GLN:HE21	1:H:62:ARG:HH21	1.59	0.51
1:H:79:TRP:CZ2	1:H:118:LYS:HB3	2.45	0.51
1:H:99:GLU:CG	1:H:128:ASN:HB2	2.38	0.51
1:D:67:LEU:HD12	1:D:67:LEU:N	2.25	0.51
1:D:304:THR:CG2	1:D:335:ARG:HD3	2.41	0.51
1:D:336:LYS:HD2	1:D:336:LYS:O	2.10	0.51
1:E:84:LYS:O	1:E:87:HIS:HB3	2.11	0.51
1:E:153:LEU:HD13	1:E:313:MET:HE1	1.92	0.51
1:F:165:ILE:HG13	1:F:170:ALA:HB1	1.93	0.51
1:F:304:THR:HG22	1:F:335:ARG:HD3	1.92	0.51
1:G:138:ALA:HB1	1:G:163:VAL:CG1	2.40	0.51
1:H:198:TYR:HB3	1:H:200:PHE:HE1	1.75	0.51
1:E:163:VAL:HG22	1:E:165:ILE:HD11	1.92	0.51
1:E:166:TYR:CD2	1:G:64:ILE:HG21	2.45	0.51
1:H:20:GLY:HA3	1:H:340:TRP:CZ2	2.45	0.51
1:F:110:LEU:HB2	1:F:177:ARG:CG	2.36	0.51
1:F:286:ASP:HB3	1:F:289:ILE:CG2	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ALA:O	1:H:22:ALA:CA	2.58	0.51
1:H:75:ILE:HA	1:H:111:ASN:HD21	1.75	0.51
1:H:76:ILE:N	1:H:115:ASN:HD21	1.96	0.51
1:D:299:MET:HB3	1:D:304:THR:HG23	1.91	0.51
1:D:357:ILE:CD1	1:D:370:VAL:HG23	2.41	0.51
1:E:153:LEU:HA	1:E:161:HIS:O	2.11	0.51
1:E:192:ILE:HD12	1:E:253:GLU:HB3	1.93	0.51
1:E:355:MET:O	1:E:373:LYS:HE3	2.11	0.51
1:F:186:THR:HG22	1:F:190:MET:HE2	1.93	0.51
1:G:330:ILE:O	1:G:332:PRO:HD3	2.10	0.51
1:H:34:ILE:C	1:H:34:ILE:HD12	2.31	0.51
1:E:122:ILE:HG22	1:E:123:MET:HE2	1.93	0.51
1:F:108:ALA:HA	1:F:137:GLN:HG2	1.93	0.51
1:F:221:LEU:CB	1:F:315:LYS:HE2	2.41	0.51
1:F:242:LEU:HD12	1:F:242:LEU:C	2.31	0.51
1:F:325:MET:SD	1:H:244:ASP:OD1	2.69	0.51
1:G:7:ALA:O	1:G:22:ALA:CA	2.59	0.51
1:G:258:PRO:HA	1:G:261:LEU:HD12	1.93	0.51
1:H:20:GLY:CA	1:H:340:TRP:HZ2	2.23	0.51
1:H:369:ILE:HG13	1:H:372:ARG:NH2	2.26	0.51
1:D:241:GLU:OE1	1:D:247:VAL:HG22	2.11	0.51
1:E:181:ALA:HB3	1:E:184:ASP:OD1	2.11	0.51
1:F:121:GLN:O	1:F:125:GLU:HG2	2.11	0.51
1:H:357:ILE:HD12	1:H:370:VAL:HG23	1.93	0.51
1:D:91:TYR:O	1:D:92:ASN:HB3	2.11	0.50
1:E:75:ILE:HA	1:E:111:ASN:HD21	1.75	0.50
1:G:44:MET:CE	1:G:45:VAL:H	2.24	0.50
1:G:102:PRO:HB2	1:G:356:TRP:HZ3	1.76	0.50
1:H:277:THR:HA	1:H:280:ASN:ND2	2.25	0.50
1:F:66:THR:HG23	1:F:203:THR:CG2	2.30	0.50
1:F:111:ASN:CG	1:F:112:PRO:HD2	2.32	0.50
1:F:219:VAL:O	1:F:220:ALA:HB3	2.11	0.50
1:F:229:THR:HG23	1:F:230:ALA:N	2.25	0.50
1:G:59:GLN:HE21	1:G:62:ARG:HH21	1.58	0.50
1:G:273:GLY:N	1:G:277:THR:HG23	2.20	0.50
1:G:349:LEU:HB3	1:G:352:PHE:CD2	2.46	0.50
1:H:120:THR:O	1:H:124:PHE:HB2	2.12	0.50
1:D:7:ALA:O	1:D:22:ALA:CA	2.59	0.50
1:D:198:TYR:HB3	1:D:200:PHE:HE1	1.77	0.50
1:E:221:LEU:CB	1:E:315:LYS:HE2	2.40	0.50
1:E:357:ILE:CD1	1:E:370:VAL:HG23	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ASN:HB3	1:F:81:ASP:OD1	2.11	0.50
1:F:302:GLY:C	1:F:304:THR:N	2.63	0.50
1:F:357:ILE:CD1	1:F:370:VAL:HG23	2.41	0.50
1:F:370:VAL:O	1:F:374:CYS:SG	2.70	0.50
1:G:153:LEU:HD13	1:G:313:MET:HE1	1.93	0.50
1:G:185:LEU:C	1:G:185:LEU:HD13	2.32	0.50
1:G:198:TYR:HB3	1:G:200:PHE:HE1	1.76	0.50
1:D:192:ILE:HD12	1:D:253:GLU:HB3	1.93	0.50
1:E:169:TYR:HA	1:G:42:GLY:CA	2.36	0.50
1:F:153:LEU:HD13	1:F:313:MET:HE1	1.94	0.50
1:F:369:ILE:HG13	1:F:372:ARG:NH2	2.27	0.50
1:G:273:GLY:H	1:G:277:THR:CG2	2.19	0.50
1:H:202:THR:CG2	1:H:205:GLU:HB2	2.35	0.50
1:D:163:VAL:HG22	1:D:165:ILE:CD1	2.42	0.50
1:D:323:SER:O	1:D:324:THR:OG1	2.24	0.50
1:E:102:PRO:HB2	1:E:356:TRP:HZ3	1.76	0.50
1:F:120:THR:O	1:F:124:PHE:HB2	2.12	0.50
1:F:139:VAL:HG21	1:H:43:VAL:HG21	1.94	0.50
1:F:340:TRP:CE3	1:F:341:ILE:HD13	2.42	0.50
1:G:163:VAL:HG22	1:G:165:ILE:HD11	1.93	0.50
1:H:111:ASN:CG	1:H:112:PRO:HD2	2.32	0.50
1:D:112:PRO:HA	1:E:194:THR:O	2.11	0.50
1:E:147:ARG:HH22	1:E:330:ILE:HD13	1.77	0.50
1:F:143:TYR:CE1	1:H:44:MET:SD	3.04	0.50
1:F:202:THR:HG22	1:F:205:GLU:N	2.17	0.50
1:H:71:ILE:HD12	1:H:76:ILE:CG1	2.38	0.50
1:E:340:TRP:CE3	1:E:341:ILE:HD13	2.41	0.50
1:G:272:ALA:HB1	1:G:277:THR:HG21	1.93	0.50
1:D:78:ASN:HB3	1:D:81:ASP:OD1	2.12	0.50
1:D:225:ASN:O	1:D:229:THR:HG22	2.12	0.50
1:D:320:LEU:HD12	1:D:321:ALA:N	2.26	0.50
1:F:273:GLY:H	1:F:277:THR:CG2	2.20	0.50
1:G:163:VAL:HG13	1:G:163:VAL:O	2.11	0.50
1:H:192:ILE:HD12	1:H:253:GLU:HB3	1.93	0.50
1:H:259:GLU:CB	1:H:263:GLN:HE22	1.99	0.50
1:H:272:ALA:HB1	1:H:277:THR:HG21	1.93	0.50
1:H:330:ILE:O	1:H:332:PRO:HD3	2.12	0.50
1:D:44:MET:HE2	1:D:45:VAL:H	1.76	0.50
1:D:272:ALA:HB1	1:D:277:THR:HG21	1.94	0.50
1:E:202:THR:HG22	1:E:205:GLU:N	2.16	0.50
1:E:302:GLY:C	1:E:304:THR:N	2.64	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:LEU:CB	1:F:177:ARG:HG3	2.36	0.50
1:F:332:PRO:HB2	1:F:334:GLU:CD	2.32	0.50
1:G:298:VAL:HG23	1:G:330:ILE:O	2.12	0.50
1:H:181:ALA:HB3	1:H:184:ASP:OD1	2.12	0.50
1:H:186:THR:O	1:H:189:LEU:HB2	2.11	0.50
1:H:226:GLU:HA	1:H:229:THR:CG2	2.41	0.50
1:D:165:ILE:HG13	1:D:170:ALA:HB1	1.94	0.49
1:D:349:LEU:HB3	1:D:352:PHE:CD2	2.46	0.49
1:F:163:VAL:HG22	1:F:165:ILE:HD11	1.94	0.49
1:G:186:THR:O	1:G:189:LEU:HB2	2.12	0.49
1:H:121:GLN:O	1:H:125:GLU:HG2	2.11	0.49
1:H:165:ILE:HG13	1:H:170:ALA:HB1	1.90	0.49
1:D:110:LEU:HB2	1:D:177:ARG:CG	2.35	0.49
1:D:136:ILE:HD13	1:D:138:ALA:N	2.26	0.49
1:D:298:VAL:HG23	1:D:330:ILE:O	2.12	0.49
1:E:111:ASN:CG	1:E:112:PRO:HD2	2.32	0.49
1:E:258:PRO:HA	1:E:261:LEU:HD12	1.94	0.49
1:G:44:MET:HE2	1:G:47:MET:HG2	1.93	0.49
1:H:370:VAL:O	1:H:374:CYS:SG	2.70	0.49
1:D:151:ILE:HG12	1:D:164:PRO:HA	1.94	0.49
1:D:219:VAL:HG23	1:D:220:ALA:N	2.26	0.49
1:E:219:VAL:O	1:E:220:ALA:HB3	2.11	0.49
1:G:62:ARG:HE	1:G:208:ILE:HD11	1.77	0.49
1:G:267:ILE:O	1:G:267:ILE:HD13	2.11	0.49
1:G:357:ILE:HD12	1:G:370:VAL:HG23	1.94	0.49
1:G:202:THR:HG22	1:G:205:GLU:N	2.17	0.49
1:H:140:LEU:HG	1:H:343:GLY:HA2	1.94	0.49
1:D:121:GLN:O	1:D:125:GLU:HG2	2.12	0.49
1:D:143:TYR:CE1	1:F:44:MET:SD	3.05	0.49
1:E:250:ILE:O	1:E:251:GLY:O	2.30	0.49
1:F:202:THR:CG2	1:F:205:GLU:HB2	2.37	0.49
1:F:304:THR:CG2	1:F:335:ARG:HD3	2.43	0.49
1:G:88:HIS:O	1:G:91:TYR:O	2.31	0.49
1:G:99:GLU:O	1:G:130:PRO:HB3	2.11	0.49
1:G:140:LEU:HG	1:G:343:GLY:HA2	1.94	0.49
1:G:340:TRP:CE3	1:G:341:ILE:HD13	2.42	0.49
1:H:111:ASN:ND2	1:H:112:PRO:HD2	2.28	0.49
1:D:84:LYS:O	1:D:87:HIS:HB3	2.12	0.49
1:D:163:VAL:HG13	1:D:163:VAL:O	2.11	0.49
1:F:62:ARG:HE	1:F:208:ILE:HD11	1.76	0.49
1:F:181:ALA:HB3	1:F:184:ASP:OD1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:VAL:HG23	1:F:330:ILE:O	2.12	0.49
1:G:84:LYS:O	1:G:87:HIS:HB3	2.12	0.49
1:G:176:MET:O	1:G:178:LEU:HD12	2.12	0.49
1:G:185:LEU:HD13	1:G:185:LEU:O	2.12	0.49
1:G:320:LEU:HD12	1:G:321:ALA:H	1.76	0.49
1:H:304:THR:CG2	1:H:335:ARG:HD3	2.43	0.49
1:H:374:CYS:O	1:H:375:PHE:HB3	2.13	0.49
1:D:34:ILE:C	1:D:34:ILE:HD12	2.32	0.49
1:D:273:GLY:N	1:D:277:THR:HG23	2.21	0.49
1:D:355:MET:O	1:D:373:LYS:HE3	2.13	0.49
1:E:110:LEU:CB	1:E:177:ARG:HG3	2.37	0.49
1:E:111:ASN:ND2	1:E:112:PRO:HD2	2.27	0.49
1:E:143:TYR:CE1	1:G:44:MET:SD	3.05	0.49
1:F:88:HIS:O	1:F:91:TYR:O	2.31	0.49
1:G:124:PHE:O	1:G:128:ASN:HA	2.13	0.49
1:G:332:PRO:HB2	1:G:334:GLU:CD	2.32	0.49
1:H:62:ARG:HE	1:H:208:ILE:HD11	1.76	0.49
1:H:287:ILE:HG23	1:H:288:ASP:N	2.27	0.49
1:D:370:VAL:O	1:D:374:CYS:SG	2.70	0.49
1:E:370:VAL:O	1:E:374:CYS:SG	2.71	0.49
1:H:153:LEU:HA	1:H:161:HIS:O	2.12	0.49
1:H:336:LYS:O	1:H:336:LYS:HD2	2.12	0.49
1:D:202:THR:HG22	1:D:205:GLU:N	2.18	0.49
1:D:372:ARG:O	1:D:373:LYS:CB	2.61	0.49
1:E:353:GLN:N	1:E:353:GLN:HE21	2.11	0.49
1:F:138:ALA:HB1	1:F:163:VAL:CG1	2.43	0.49
1:G:245:GLY:O	1:G:246:GLN:HG3	2.12	0.49
1:G:304:THR:CG2	1:G:335:ARG:HD3	2.43	0.49
1:H:320:LEU:HD12	1:H:321:ALA:N	2.28	0.49
1:D:212:ILE:HD12	1:D:240:TYR:CE1	2.48	0.49
1:D:221:LEU:CB	1:D:315:LYS:HE2	2.41	0.49
1:E:136:ILE:HD13	1:E:136:ILE:C	2.33	0.49
1:E:140:LEU:HG	1:E:343:GLY:HA2	1.95	0.49
1:E:320:LEU:HD12	1:E:321:ALA:N	2.27	0.49
1:G:120:THR:O	1:G:124:PHE:HB2	2.13	0.49
1:G:165:ILE:HG13	1:G:170:ALA:HB1	1.94	0.49
1:G:221:LEU:CB	1:G:315:LYS:HE2	2.42	0.49
1:G:327:ILE:HD13	1:G:327:ILE:N	2.26	0.49
1:H:202:THR:HG22	1:H:205:GLU:N	2.18	0.49
1:H:327:ILE:HD13	1:H:327:ILE:N	2.26	0.49
1:D:34:ILE:O	1:D:35:VAL:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:MET:HG2	1:D:255:PHE:HE1	1.78	0.48
1:F:80:ASP:O	1:F:83:GLU:HG2	2.13	0.48
1:G:165:ILE:HD12	1:G:165:ILE:N	2.27	0.48
1:D:102:PRO:HB2	1:D:356:TRP:HZ3	1.76	0.48
1:D:357:ILE:HD12	1:D:370:VAL:HG23	1.95	0.48
1:E:23:GLY:HA2	1:E:344:SER:CB	2.37	0.48
1:F:102:PRO:HB2	1:F:356:TRP:HZ3	1.76	0.48
1:F:359:LYS:O	1:F:360:GLN:CB	2.61	0.48
1:G:263:GLN:O	1:G:263:GLN:CG	2.61	0.48
1:H:44:MET:CE	1:H:45:VAL:H	2.25	0.48
1:H:70:PRO:HB2	1:H:82:MET:SD	2.53	0.48
1:H:120:THR:O	1:H:124:PHE:CB	2.61	0.48
1:H:332:PRO:HB2	1:H:334:GLU:CD	2.33	0.48
1:D:140:LEU:HG	1:D:343:GLY:HA2	1.94	0.48
1:D:147:ARG:HH22	1:D:330:ILE:HD13	1.77	0.48
1:D:340:TRP:CE3	1:D:341:ILE:HD13	2.42	0.48
1:E:163:VAL:HG22	1:E:165:ILE:CD1	2.43	0.48
1:E:273:GLY:H	1:E:277:THR:CG2	2.17	0.48
1:E:330:ILE:O	1:E:332:PRO:HD3	2.13	0.48
1:F:100:GLU:OE2	1:F:100:GLU:N	2.45	0.48
1:F:120:THR:O	1:F:124:PHE:CB	2.61	0.48
1:F:140:LEU:HG	1:F:343:GLY:HA2	1.94	0.48
1:F:263:GLN:O	1:F:263:GLN:HG2	2.13	0.48
1:G:320:LEU:HD12	1:G:321:ALA:N	2.28	0.48
1:H:171:LEU:HD23	1:H:173:HIS:HB2	1.95	0.48
1:D:13:GLY:O	1:D:14:SER:OG	2.29	0.48
1:D:143:TYR:CE2	1:D:346:LEU:HB2	2.48	0.48
1:D:332:PRO:HB2	1:D:334:GLU:CD	2.33	0.48
1:F:165:ILE:HD12	1:F:165:ILE:N	2.28	0.48
1:H:102:PRO:CB	1:H:131:ALA:HB3	2.42	0.48
1:H:219:VAL:HG23	1:H:220:ALA:N	2.28	0.48
1:D:263:GLN:O	1:D:263:GLN:CG	2.61	0.48
1:E:298:VAL:HG23	1:E:330:ILE:O	2.13	0.48
1:F:332:PRO:O	1:F:335:ARG:HB3	2.14	0.48
1:G:219:VAL:HG23	1:G:220:ALA:N	2.28	0.48
1:H:176:MET:O	1:H:178:LEU:HD12	2.14	0.48
1:E:78:ASN:HB3	1:E:81:ASP:OD1	2.14	0.48
1:E:151:ILE:HG12	1:E:164:PRO:HA	1.94	0.48
1:G:240:TYR:CG	1:G:241:GLU:N	2.82	0.48
1:H:166:TYR:O	1:H:169:TYR:O	2.32	0.48
1:H:212:ILE:HD12	1:H:240:TYR:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:355:MET:O	1:H:373:LYS:HE3	2.12	0.48
1:D:165:ILE:HD12	1:D:165:ILE:N	2.29	0.48
1:E:187:ASP:HA	1:E:190:MET:HE3	1.95	0.48
1:H:84:LYS:O	1:H:87:HIS:HB3	2.12	0.48
1:D:355:MET:HE2	1:D:356:TRP:NE1	2.28	0.48
1:E:332:PRO:O	1:E:335:ARG:HB3	2.13	0.48
1:F:169:TYR:HA	1:H:42:GLY:CA	2.38	0.48
1:F:327:ILE:HD13	1:F:327:ILE:N	2.27	0.48
1:H:221:LEU:H	1:H:221:LEU:CD1	2.25	0.48
1:H:353:GLN:N	1:H:353:GLN:HE21	2.11	0.48
1:D:138:ALA:HB1	1:D:163:VAL:CG1	2.44	0.48
1:F:99:GLU:CG	1:F:128:ASN:HB2	2.40	0.48
1:F:240:TYR:CG	1:F:241:GLU:N	2.81	0.48
1:G:100:GLU:OE2	1:G:100:GLU:N	2.47	0.48
1:G:359:LYS:O	1:G:360:GLN:CB	2.62	0.48
1:H:138:ALA:CB	1:H:163:VAL:HG11	2.44	0.48
1:D:80:ASP:O	1:D:83:GLU:HG2	2.14	0.48
1:D:211:ASP:OD1	1:D:212:ILE:N	2.47	0.48
1:E:70:PRO:HB2	1:E:82:MET:SD	2.53	0.48
1:E:91:TYR:O	1:E:92:ASN:HB3	2.13	0.48
1:F:84:LYS:O	1:F:87:HIS:HB3	2.13	0.48
1:G:147:ARG:HH22	1:G:330:ILE:HD13	1.77	0.48
1:H:78:ASN:HB3	1:H:81:ASP:OD1	2.13	0.48
1:D:111:ASN:CG	1:D:112:PRO:HD2	2.35	0.47
1:D:369:ILE:HG13	1:D:372:ARG:HH22	1.79	0.47
1:E:143:TYR:CE2	1:E:346:LEU:HB2	2.49	0.47
1:E:176:MET:O	1:E:178:LEU:HD12	2.14	0.47
1:G:163:VAL:HG22	1:G:165:ILE:CD1	2.44	0.47
1:E:240:TYR:CG	1:E:241:GLU:N	2.82	0.47
1:F:151:ILE:HG12	1:F:164:PRO:HA	1.97	0.47
1:G:78:ASN:HB3	1:G:81:ASP:OD1	2.14	0.47
1:G:80:ASP:O	1:G:83:GLU:HG2	2.14	0.47
1:G:111:ASN:CG	1:G:112:PRO:HD2	2.34	0.47
1:G:238:LYS:HZ2	1:G:254:ARG:HH12	1.61	0.47
1:G:355:MET:HE2	1:G:356:TRP:NE1	2.29	0.47
1:H:355:MET:HE2	1:H:356:TRP:NE1	2.29	0.47
1:D:102:PRO:CB	1:D:131:ALA:HB3	2.43	0.47
1:E:43:VAL:HG13	1:E:44:MET:N	2.28	0.47
1:E:110:LEU:HB2	1:E:177:ARG:CG	2.37	0.47
1:E:327:ILE:HD13	1:E:327:ILE:N	2.28	0.47
1:F:192:ILE:HD12	1:F:253:GLU:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ASP:O	1:H:83:GLU:HG2	2.14	0.47
1:H:298:VAL:HG23	1:H:330:ILE:O	2.13	0.47
1:D:44:MET:CE	1:D:45:VAL:H	2.27	0.47
1:E:196:ARG:NH2	1:E:251:GLY:HA3	2.22	0.47
1:E:332:PRO:HB2	1:E:334:GLU:CD	2.34	0.47
1:E:374:CYS:O	1:E:375:PHE:HB3	2.14	0.47
1:F:176:MET:O	1:F:178:LEU:HD12	2.15	0.47
1:F:221:LEU:H	1:F:221:LEU:CD1	2.26	0.47
1:G:23:GLY:HA2	1:G:344:SER:CB	2.37	0.47
1:G:102:PRO:CB	1:G:131:ALA:HB3	2.43	0.47
1:G:329:ILE:O	1:G:330:ILE:C	2.53	0.47
1:H:186:THR:HG22	1:H:190:MET:HE2	1.95	0.47
1:D:73:HIS:HA	1:D:158:GLY:O	2.15	0.47
1:E:339:VAL:HG23	1:E:340:TRP:H	1.78	0.47
1:F:147:ARG:HH22	1:F:330:ILE:HD13	1.77	0.47
1:D:8:LEU:N	1:D:102:PRO:O	2.45	0.47
1:D:334:GLU:CD	1:D:334:GLU:H	2.18	0.47
1:E:34:ILE:O	1:E:35:VAL:HG13	2.15	0.47
1:E:78:ASN:HD22	1:E:81:ASP:CG	2.18	0.47
1:E:165:ILE:HD12	1:E:165:ILE:N	2.29	0.47
1:E:227:MET:HG2	1:E:255:PHE:HE1	1.78	0.47
1:F:139:VAL:HG22	1:H:43:VAL:HG11	1.95	0.47
1:F:227:MET:HG2	1:F:255:PHE:HE1	1.79	0.47
1:F:259:GLU:CB	1:F:263:GLN:HE22	2.01	0.47
1:G:138:ALA:CB	1:G:163:VAL:HG11	2.45	0.47
1:H:238:LYS:HD3	1:H:239:SER:O	2.14	0.47
1:H:287:ILE:CG2	1:H:288:ASP:N	2.78	0.47
1:H:361:GLU:H	1:H:361:GLU:HG3	1.42	0.47
1:D:129:VAL:HG21	1:D:132:MET:CG	2.40	0.47
1:D:325:MET:SD	1:F:244:ASP:OD1	2.73	0.47
1:D:329:ILE:CD1	1:D:329:ILE:N	2.73	0.47
1:E:136:ILE:HD13	1:E:138:ALA:N	2.29	0.47
1:E:138:ALA:HB1	1:E:163:VAL:CG1	2.44	0.47
1:E:171:LEU:HD23	1:E:173:HIS:HB2	1.97	0.47
1:E:263:GLN:O	1:E:263:GLN:CG	2.63	0.47
1:F:111:ASN:ND2	1:F:112:PRO:HD2	2.30	0.47
1:F:202:THR:HG23	1:F:204:ALA:H	1.80	0.47
1:F:330:ILE:O	1:F:332:PRO:HD3	2.15	0.47
1:F:357:ILE:HD12	1:F:370:VAL:HG23	1.96	0.47
1:G:99:GLU:CG	1:G:128:ASN:HB2	2.43	0.47
1:G:120:THR:O	1:G:124:PHE:CB	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ILE:HD12	1:G:253:GLU:HB3	1.97	0.47
1:H:73:HIS:HA	1:H:158:GLY:O	2.15	0.47
1:D:176:MET:O	1:D:178:LEU:HD12	2.14	0.47
1:E:120:THR:O	1:E:124:PHE:HB2	2.15	0.47
1:F:22:ALA:HB1	1:F:348:SER:HB2	1.97	0.47
1:F:136:ILE:HD13	1:F:136:ILE:C	2.35	0.47
1:F:163:VAL:HG13	1:F:163:VAL:O	2.15	0.47
1:F:163:VAL:HG22	1:F:165:ILE:CD1	2.45	0.47
1:G:34:ILE:C	1:G:34:ILE:HD12	2.34	0.47
1:G:211:ASP:HA	1:G:214:GLU:HG3	1.96	0.47
1:G:238:LYS:HD3	1:G:239:SER:O	2.15	0.47
1:H:124:PHE:O	1:H:128:ASN:HA	2.15	0.47
1:D:332:PRO:O	1:D:335:ARG:HB3	2.15	0.47
1:E:139:VAL:CG2	1:G:43:VAL:HG11	2.45	0.47
1:H:320:LEU:HD12	1:H:321:ALA:H	1.80	0.47
1:D:7:ALA:N	1:D:22:ALA:HB2	2.22	0.47
1:E:163:VAL:HG13	1:E:163:VAL:O	2.15	0.47
1:E:238:LYS:HZ2	1:E:254:ARG:HH12	1.63	0.47
1:E:325:MET:SD	1:G:244:ASP:OD1	2.73	0.47
1:E:357:ILE:HD12	1:E:370:VAL:HG23	1.96	0.47
1:G:147:ARG:CZ	1:G:330:ILE:HD13	2.45	0.47
1:G:230:ALA:O	1:G:233:SER:O	2.33	0.47
1:H:25:ASP:O	1:H:26:ALA:O	2.33	0.47
1:H:211:ASP:OD1	1:H:212:ILE:N	2.48	0.47
1:H:295:ALA:HB1	1:H:328:LYS:NZ	2.30	0.47
1:H:300:SER:HA	1:H:335:ARG:HB2	1.97	0.47
1:D:70:PRO:HB2	1:D:82:MET:SD	2.56	0.46
1:D:192:ILE:HD12	1:D:253:GLU:CB	2.45	0.46
1:E:34:ILE:HD12	1:E:34:ILE:C	2.35	0.46
1:E:202:THR:HG23	1:E:204:ALA:H	1.79	0.46
1:F:171:LEU:HD23	1:F:173:HIS:HB2	1.97	0.46
1:H:54:VAL:HG11	1:H:88:HIS:CB	2.45	0.46
1:H:100:GLU:OE2	1:H:100:GLU:N	2.48	0.46
1:D:111:ASN:ND2	1:D:112:PRO:HD2	2.29	0.46
1:G:334:GLU:CD	1:G:334:GLU:H	2.18	0.46
1:H:138:ALA:CB	1:H:163:VAL:CG1	2.94	0.46
1:H:245:GLY:O	1:H:246:GLN:HG3	2.16	0.46
1:H:263:GLN:O	1:H:263:GLN:CG	2.62	0.46
1:D:374:CYS:O	1:D:375:PHE:HB3	2.15	0.46
1:F:361:GLU:H	1:F:361:GLU:HG3	1.40	0.46
1:G:339:VAL:HG23	1:G:340:TRP:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:ILE:O	1:H:35:VAL:HG13	2.14	0.46
1:H:238:LYS:HZ2	1:H:254:ARG:HH12	1.62	0.46
1:D:43:VAL:HG13	1:D:44:MET:N	2.31	0.46
1:D:178:LEU:H	1:D:178:LEU:CD1	2.22	0.46
1:D:211:ASP:HA	1:D:214:GLU:HG3	1.97	0.46
1:F:211:ASP:HA	1:F:214:GLU:HG3	1.95	0.46
1:F:329:ILE:O	1:F:330:ILE:C	2.54	0.46
1:G:287:ILE:HG23	1:G:288:ASP:N	2.29	0.46
1:G:353:GLN:HE21	1:G:353:GLN:N	2.13	0.46
1:H:147:ARG:HH22	1:H:330:ILE:HD13	1.78	0.46
1:D:147:ARG:CZ	1:D:330:ILE:HD13	2.45	0.46
1:D:240:TYR:CG	1:D:241:GLU:N	2.83	0.46
1:E:113:LYS:HG2	1:E:117:GLU:CD	2.36	0.46
1:E:211:ASP:OD1	1:E:212:ILE:N	2.48	0.46
1:E:372:ARG:O	1:E:373:LYS:CB	2.64	0.46
1:G:25:ASP:O	1:G:26:ALA:O	2.34	0.46
1:H:202:THR:HG23	1:H:204:ALA:H	1.81	0.46
1:D:25:ASP:O	1:D:26:ALA:O	2.34	0.46
1:E:53:TYR:C	1:E:54:VAL:HG22	2.36	0.46
1:E:120:THR:O	1:E:124:PHE:CB	2.64	0.46
1:E:121:GLN:O	1:E:125:GLU:HG2	2.16	0.46
1:E:211:ASP:HA	1:E:214:GLU:HG3	1.98	0.46
1:F:75:ILE:HG12	1:F:111:ASN:OD1	2.15	0.46
1:F:124:PHE:O	1:F:128:ASN:HA	2.16	0.46
1:F:143:TYR:CE2	1:F:346:LEU:HB2	2.50	0.46
1:F:213:LYS:O	1:F:217:CYS:HB3	2.16	0.46
1:G:22:ALA:HB1	1:G:348:SER:HB2	1.98	0.46
1:G:111:ASN:ND2	1:G:112:PRO:HD2	2.30	0.46
1:H:323:SER:O	1:H:324:THR:OG1	2.28	0.46
1:D:23:GLY:HA2	1:D:344:SER:CB	2.38	0.46
1:D:78:ASN:HD22	1:D:81:ASP:CG	2.19	0.46
1:D:202:THR:HG23	1:D:204:ALA:H	1.81	0.46
1:D:273:GLY:H	1:D:277:THR:CG2	2.22	0.46
1:E:124:PHE:O	1:E:128:ASN:HA	2.16	0.46
1:E:163:VAL:HG13	1:E:165:ILE:HD11	1.98	0.46
1:F:13:GLY:O	1:F:14:SER:OG	2.26	0.46
1:F:99:GLU:O	1:F:130:PRO:HB3	2.15	0.46
1:G:196:ARG:NH2	1:G:251:GLY:HA3	2.25	0.46
1:H:196:ARG:NH2	1:H:251:GLY:HA3	2.23	0.46
1:H:219:VAL:O	1:H:220:ALA:HB3	2.16	0.46
1:D:139:VAL:HG22	1:F:43:VAL:HG11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:VAL:HG13	1:D:165:ILE:HD11	1.98	0.46
1:E:80:ASP:O	1:E:83:GLU:HG2	2.16	0.46
1:F:104:LEU:HD12	1:F:133:TYR:O	2.16	0.46
1:F:355:MET:HE2	1:F:356:TRP:NE1	2.31	0.46
1:G:117:GLU:OE2	1:G:371:HIS:HB2	2.16	0.46
1:H:91:TYR:O	1:H:92:ASN:HB3	2.16	0.46
1:D:124:PHE:O	1:D:128:ASN:HA	2.16	0.46
1:E:147:ARG:CZ	1:E:330:ILE:HD13	2.46	0.46
1:G:104:LEU:HD12	1:G:133:TYR:O	2.15	0.46
1:G:287:ILE:CG2	1:G:288:ASP:N	2.78	0.46
1:D:136:ILE:HD13	1:D:139:VAL:H	1.80	0.46
1:E:100:GLU:OE2	1:E:100:GLU:N	2.49	0.46
1:E:104:LEU:HD12	1:E:133:TYR:O	2.15	0.46
1:F:163:VAL:HG13	1:F:165:ILE:HD11	1.98	0.46
1:F:230:ALA:O	1:F:233:SER:O	2.34	0.46
1:G:54:VAL:HG11	1:G:88:HIS:CB	2.46	0.46
1:H:211:ASP:HA	1:H:214:GLU:HG3	1.97	0.46
1:H:230:ALA:O	1:H:233:SER:O	2.34	0.46
1:H:359:LYS:O	1:H:360:GLN:CB	2.64	0.46
1:D:309:ILE:HD13	1:D:309:ILE:HA	1.81	0.45
1:E:5:THR:OG1	1:E:101:HIS:HA	2.16	0.45
1:E:54:VAL:HG11	1:E:88:HIS:CB	2.47	0.45
1:E:136:ILE:HD12	1:E:139:VAL:CG2	2.39	0.45
1:F:34:ILE:O	1:F:35:VAL:HG13	2.16	0.45
1:F:73:HIS:HA	1:F:158:GLY:O	2.16	0.45
1:F:238:LYS:HZ2	1:F:254:ARG:HH12	1.63	0.45
1:F:374:CYS:O	1:F:375:PHE:HB3	2.17	0.45
1:G:11:ASP:CB	1:G:18:LYS:HB2	2.46	0.45
1:G:332:PRO:O	1:G:335:ARG:HB3	2.16	0.45
1:H:11:ASP:HB2	1:H:18:LYS:HB2	1.98	0.45
1:H:227:MET:HG2	1:H:255:PHE:HE1	1.79	0.45
1:H:242:LEU:HG	1:H:246:GLN:C	2.37	0.45
1:H:302:GLY:C	1:H:304:THR:N	2.63	0.45
1:D:5:THR:OG1	1:D:101:HIS:HA	2.16	0.45
1:D:52:SER:O	1:D:53:TYR:CD1	2.69	0.45
1:D:334:GLU:OE2	1:D:334:GLU:N	2.47	0.45
1:D:339:VAL:HG23	1:D:340:TRP:H	1.80	0.45
1:E:25:ASP:O	1:E:26:ALA:O	2.35	0.45
1:E:75:ILE:HG12	1:E:111:ASN:OD1	2.15	0.45
1:E:105:LEU:HD22	1:E:105:LEU:N	2.31	0.45
1:E:192:ILE:HD12	1:E:253:GLU:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:LEU:HD12	1:F:21:PHE:HA	1.98	0.45
1:F:245:GLY:O	1:F:246:GLN:HG3	2.17	0.45
1:F:353:GLN:N	1:F:353:GLN:HE21	2.14	0.45
1:E:147:ARG:NH2	1:E:330:ILE:HD13	2.32	0.45
1:E:212:ILE:HD12	1:E:240:TYR:CE1	2.51	0.45
1:F:25:ASP:O	1:F:26:ALA:O	2.33	0.45
1:F:71:ILE:HD12	1:F:76:ILE:CG1	2.38	0.45
1:F:209:VAL:C	1:F:212:ILE:HG12	2.36	0.45
1:F:238:LYS:HD3	1:F:239:SER:O	2.17	0.45
1:G:138:ALA:CB	1:G:163:VAL:CG1	2.94	0.45
1:G:221:LEU:H	1:G:221:LEU:CD1	2.28	0.45
1:H:113:LYS:HG2	1:H:117:GLU:CD	2.37	0.45
1:H:163:VAL:HG13	1:H:163:VAL:O	2.16	0.45
1:H:329:ILE:O	1:H:330:ILE:C	2.55	0.45
1:H:370:VAL:HG13	1:H:371:HIS:N	2.31	0.45
1:D:136:ILE:HD13	1:D:136:ILE:C	2.37	0.45
1:D:287:ILE:CG2	1:D:288:ASP:N	2.79	0.45
1:E:71:ILE:HD12	1:E:76:ILE:CG1	2.38	0.45
1:E:99:GLU:O	1:E:130:PRO:HB3	2.16	0.45
1:G:8:LEU:HD12	1:G:21:PHE:HA	1.98	0.45
1:G:70:PRO:HB2	1:G:82:MET:SD	2.56	0.45
1:D:8:LEU:HD12	1:D:21:PHE:HA	1.97	0.45
1:D:275:HIS:H	1:D:275:HIS:CD2	2.34	0.45
1:E:221:LEU:H	1:E:221:LEU:CD1	2.22	0.45
1:F:325:MET:CE	1:F:326:LYS:H	2.29	0.45
1:G:334:GLU:OE2	1:G:334:GLU:N	2.47	0.45
1:H:99:GLU:O	1:H:130:PRO:HB3	2.17	0.45
1:D:105:LEU:HD22	1:D:105:LEU:N	2.30	0.45
1:F:136:ILE:HD13	1:F:139:VAL:H	1.82	0.45
1:F:309:ILE:HA	1:F:309:ILE:HD13	1.80	0.45
1:F:346:LEU:HD11	1:F:355:MET:HE1	1.98	0.45
1:G:37:ARG:HB3	1:G:38:PRO:HD2	1.97	0.45
1:G:121:GLN:HA	1:G:125:GLU:HG2	1.97	0.45
1:H:176:MET:HE1	1:H:277:THR:C	2.36	0.45
1:D:11:ASP:HB2	1:D:18:LYS:HB2	1.98	0.45
1:D:140:LEU:N	1:D:140:LEU:CD1	2.79	0.45
1:D:330:ILE:O	1:D:332:PRO:HD3	2.16	0.45
1:E:92:ASN:ND2	1:E:93:GLU:HG3	2.32	0.45
1:E:334:GLU:CD	1:E:334:GLU:H	2.20	0.45
1:F:92:ASN:ND2	1:F:93:GLU:HG3	2.31	0.45
1:H:8:LEU:HD12	1:H:21:PHE:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:ILE:HD12	1:H:253:GLU:CB	2.46	0.45
1:H:334:GLU:N	1:H:334:GLU:OE2	2.48	0.45
1:D:267:ILE:CG2	1:D:268:GLY:N	2.79	0.45
1:D:287:ILE:HG23	1:D:288:ASP:N	2.30	0.45
1:E:200:PHE:HA	1:E:205:GLU:OE1	2.17	0.45
1:F:147:ARG:CZ	1:F:330:ILE:HD13	2.45	0.45
1:G:11:ASP:HB2	1:G:18:LYS:HB2	1.98	0.45
1:G:211:ASP:OD1	1:G:212:ILE:N	2.50	0.45
1:D:22:ALA:HB1	1:D:348:SER:HB2	1.99	0.45
1:D:53:TYR:C	1:D:54:VAL:HG22	2.37	0.45
1:D:113:LYS:HG2	1:D:117:GLU:CD	2.37	0.45
1:E:44:MET:CE	1:E:45:VAL:H	2.30	0.45
1:E:176:MET:HE1	1:E:277:THR:C	2.37	0.45
1:F:61:LYS:CB	1:F:64:ILE:HD11	2.47	0.45
1:F:139:VAL:CG2	1:H:43:VAL:HG11	2.47	0.45
1:G:147:ARG:NH2	1:G:330:ILE:HD13	2.31	0.45
1:G:171:LEU:HD23	1:G:173:HIS:HB2	1.99	0.45
1:G:369:ILE:HG13	1:G:372:ARG:HH22	1.82	0.45
1:E:275:HIS:CD2	1:E:275:HIS:H	2.35	0.45
1:E:369:ILE:HG13	1:E:372:ARG:HH22	1.80	0.45
1:F:70:PRO:HB2	1:F:82:MET:SD	2.57	0.45
1:F:78:ASN:HD22	1:F:81:ASP:CG	2.20	0.45
1:F:166:TYR:HD2	1:H:64:ILE:HG21	1.82	0.45
1:G:257:CYS:SG	1:G:258:PRO:N	2.90	0.45
1:H:121:GLN:HA	1:H:125:GLU:HG2	1.98	0.45
1:H:334:GLU:CD	1:H:334:GLU:H	2.21	0.45
1:D:117:GLU:OE2	1:D:371:HIS:HB2	2.17	0.44
1:D:171:LEU:HD23	1:D:173:HIS:HB2	2.00	0.44
1:D:277:THR:HA	1:D:280:ASN:HD22	1.82	0.44
1:E:312:ARG:HA	1:E:315:LYS:HE3	2.00	0.44
1:F:23:GLY:HA2	1:F:344:SER:CB	2.35	0.44
1:F:176:MET:HE1	1:F:277:THR:C	2.37	0.44
1:F:334:GLU:CD	1:F:334:GLU:H	2.21	0.44
1:G:160:THR:OG1	1:G:178:LEU:HD13	2.18	0.44
1:G:242:LEU:HG	1:G:246:GLN:C	2.35	0.44
1:G:300:SER:HA	1:G:335:ARG:HB2	1.99	0.44
1:D:110:LEU:CB	1:D:177:ARG:HG3	2.36	0.44
1:E:250:ILE:H	1:E:250:ILE:HD12	1.82	0.44
1:F:11:ASP:CB	1:F:18:LYS:HB2	2.47	0.44
1:F:113:LYS:HG2	1:F:117:GLU:CD	2.38	0.44
1:F:211:ASP:OD1	1:F:212:ILE:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:ASP:O	1:G:4:GLU:O	2.34	0.44
1:G:98:PRO:HG3	1:G:127:PHE:HD1	1.83	0.44
1:G:289:ILE:C	1:G:289:ILE:HD13	2.38	0.44
1:H:339:VAL:HG23	1:H:340:TRP:H	1.79	0.44
1:D:11:ASP:CB	1:D:18:LYS:HB2	2.47	0.44
1:D:142:LEU:HD21	1:D:165:ILE:HB	1.98	0.44
1:G:136:ILE:HD13	1:G:136:ILE:C	2.37	0.44
1:G:142:LEU:HD21	1:G:165:ILE:HB	1.98	0.44
1:G:212:ILE:HD12	1:G:240:TYR:CE1	2.52	0.44
1:H:23:GLY:HA2	1:H:344:SER:CB	2.36	0.44
1:H:66:THR:HA	1:H:203:THR:OG1	2.18	0.44
1:H:89:THR:O	1:H:94:LEU:HG	2.17	0.44
1:H:136:ILE:HD13	1:H:139:VAL:H	1.81	0.44
1:H:160:THR:OG1	1:H:178:LEU:HD13	2.18	0.44
1:H:326:LYS:HE3	1:H:327:ILE:N	2.32	0.44
1:F:54:VAL:HG11	1:F:88:HIS:CB	2.47	0.44
1:F:138:ALA:CB	1:F:163:VAL:HG11	2.48	0.44
1:F:370:VAL:HG13	1:F:371:HIS:N	2.31	0.44
1:G:227:MET:HG2	1:G:255:PHE:HE1	1.81	0.44
1:G:249:THR:HG23	1:G:249:THR:O	2.18	0.44
1:H:61:LYS:CB	1:H:64:ILE:HD11	2.48	0.44
1:H:92:ASN:ND2	1:H:93:GLU:HG3	2.32	0.44
1:H:147:ARG:CZ	1:H:330:ILE:HD13	2.45	0.44
1:H:277:THR:O	1:H:280:ASN:ND2	2.51	0.44
1:H:332:PRO:O	1:H:335:ARG:HB3	2.18	0.44
1:D:147:ARG:NH2	1:D:330:ILE:HD13	2.32	0.44
1:D:176:MET:HE1	1:D:277:THR:C	2.38	0.44
1:D:188:TYR:O	1:D:192:ILE:HG23	2.17	0.44
1:D:353:GLN:N	1:D:353:GLN:HE21	2.16	0.44
1:D:359:LYS:O	1:D:360:GLN:CB	2.64	0.44
1:E:121:GLN:HA	1:E:125:GLU:HG2	1.99	0.44
1:E:349:LEU:HB3	1:E:352:PHE:HE2	1.82	0.44
1:F:117:GLU:OE2	1:F:371:HIS:HB2	2.17	0.44
1:F:129:VAL:HG21	1:F:132:MET:CG	2.38	0.44
1:H:11:ASP:CB	1:H:18:LYS:HB2	2.47	0.44
1:H:111:ASN:CG	1:H:112:PRO:CD	2.86	0.44
1:H:117:GLU:OE2	1:H:371:HIS:HB2	2.17	0.44
1:H:151:ILE:HG12	1:H:164:PRO:HA	2.00	0.44
1:H:214:GLU:HG2	2:H:401:ADP:C2	2.53	0.44
1:F:312:ARG:HA	1:F:315:LYS:HE3	1.99	0.44
1:F:334:GLU:N	1:F:334:GLU:OE2	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:OE2	1:D:100:GLU:N	2.50	0.44
1:D:196:ARG:NH2	1:D:251:GLY:HA3	2.23	0.44
1:D:361:GLU:O	1:D:364:GLU:HG2	2.18	0.44
1:E:64:ILE:H	1:E:64:ILE:HG13	1.55	0.44
1:E:277:THR:HA	1:E:280:ASN:HD22	1.83	0.44
1:F:214:GLU:HG2	2:F:401:ADP:C2	2.53	0.44
1:F:250:ILE:H	1:F:250:ILE:HD12	1.82	0.44
1:G:53:TYR:C	1:G:54:VAL:HG22	2.38	0.44
1:G:124:PHE:CZ	1:G:359:LYS:HA	2.53	0.44
1:H:5:THR:OG1	1:H:101:HIS:HA	2.17	0.44
1:H:349:LEU:HB3	1:H:352:PHE:HE2	1.82	0.44
1:D:54:VAL:HG11	1:D:88:HIS:CB	2.48	0.44
1:D:325:MET:CE	1:D:326:LYS:H	2.31	0.44
1:D:329:ILE:O	1:D:330:ILE:C	2.55	0.44
1:E:214:GLU:HG2	2:E:401:ADP:C2	2.53	0.44
1:G:61:LYS:CB	1:G:64:ILE:HD11	2.48	0.44
1:G:71:ILE:HD12	1:G:76:ILE:CG1	2.40	0.44
1:G:73:HIS:HA	1:G:158:GLY:O	2.17	0.44
1:G:202:THR:HG23	1:G:204:ALA:H	1.83	0.44
1:H:147:ARG:NH2	1:H:330:ILE:HD13	2.32	0.44
1:D:259:GLU:CB	1:D:263:GLN:HE22	2.00	0.44
1:D:300:SER:HA	1:D:335:ARG:HB2	2.00	0.44
1:E:111:ASN:CG	1:E:112:PRO:CD	2.87	0.44
1:E:138:ALA:CB	1:E:163:VAL:HG11	2.48	0.44
1:F:105:LEU:HD22	1:F:105:LEU:N	2.31	0.44
1:F:166:TYR:O	1:F:169:TYR:O	2.36	0.44
1:F:249:THR:HG23	1:F:249:THR:O	2.16	0.44
1:F:277:THR:HA	1:F:280:ASN:HD22	1.83	0.44
1:F:352:PHE:HZ	1:H:47:MET:CE	2.30	0.44
1:H:22:ALA:HB1	1:H:348:SER:HB2	2.00	0.44
1:H:275:HIS:H	1:H:275:HIS:CD2	2.34	0.44
1:D:245:GLY:O	1:D:246:GLN:HG3	2.18	0.43
1:D:330:ILE:O	1:D:330:ILE:CG2	2.64	0.43
1:E:326:LYS:HE3	1:E:327:ILE:N	2.33	0.43
1:E:346:LEU:HD11	1:E:355:MET:HE1	2.00	0.43
1:E:355:MET:HE2	1:E:356:TRP:NE1	2.31	0.43
1:F:121:GLN:HA	1:F:125:GLU:HG2	2.00	0.43
1:F:212:ILE:HD12	1:F:240:TYR:CE1	2.53	0.43
1:F:280:ASN:OD1	1:F:281:SER:N	2.50	0.43
1:G:92:ASN:ND2	1:G:93:GLU:HG3	2.33	0.43
1:G:110:LEU:HB2	1:G:177:ARG:CG	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:MET:HE1	1:G:277:THR:CB	2.38	0.43
1:G:213:LYS:O	1:G:217:CYS:HB3	2.18	0.43
1:D:92:ASN:ND2	1:D:93:GLU:HG3	2.32	0.43
1:D:163:VAL:CG2	1:D:165:ILE:HD11	2.48	0.43
1:E:61:LYS:CB	1:E:64:ILE:HD11	2.48	0.43
1:E:76:ILE:CG2	1:E:79:TRP:H	2.31	0.43
1:E:200:PHE:O	1:E:201:VAL:HG13	2.18	0.43
1:E:229:THR:HG23	1:E:230:ALA:H	1.82	0.43
1:G:78:ASN:HD22	1:G:81:ASP:CG	2.22	0.43
1:G:136:ILE:HD13	1:G:139:VAL:H	1.82	0.43
1:G:372:ARG:O	1:G:373:LYS:CB	2.65	0.43
1:H:163:VAL:HG13	1:H:165:ILE:HD11	2.00	0.43
1:H:206:ARG:HA	1:H:209:VAL:HG12	2.00	0.43
1:H:240:TYR:CG	1:H:241:GLU:N	2.86	0.43
1:H:372:ARG:O	1:H:373:LYS:CB	2.65	0.43
1:D:22:ALA:O	1:D:23:GLY:C	2.57	0.43
1:E:11:ASP:CB	1:E:18:LYS:HB2	2.48	0.43
1:E:209:VAL:C	1:E:212:ILE:HG12	2.37	0.43
1:E:287:ILE:HG23	1:E:288:ASP:N	2.33	0.43
1:F:11:ASP:HB2	1:F:18:LYS:HB2	1.98	0.43
1:F:147:ARG:NH2	1:F:330:ILE:HD13	2.32	0.43
1:G:5:THR:OG1	1:G:101:HIS:HA	2.18	0.43
1:G:75:ILE:HG12	1:G:111:ASN:OD1	2.17	0.43
1:G:209:VAL:C	1:G:212:ILE:HG12	2.38	0.43
1:H:138:ALA:HB1	1:H:163:VAL:HG12	2.00	0.43
1:H:163:VAL:CG2	1:H:165:ILE:HD11	2.47	0.43
1:H:188:TYR:O	1:H:192:ILE:HG23	2.18	0.43
1:D:75:ILE:HG12	1:D:111:ASN:OD1	2.18	0.43
1:E:166:TYR:HD2	1:G:64:ILE:HG21	1.83	0.43
1:E:330:ILE:O	1:E:330:ILE:CG2	2.65	0.43
1:F:11:ASP:O	1:F:106:THR:HB	2.18	0.43
1:F:95:ARG:CZ	1:F:95:ARG:HB2	2.49	0.43
1:F:279:TYR:O	1:F:282:ILE:HG22	2.19	0.43
1:F:287:ILE:HG23	1:F:288:ASP:N	2.32	0.43
1:F:369:ILE:HG13	1:F:372:ARG:HH22	1.83	0.43
1:G:105:LEU:HD22	1:G:105:LEU:N	2.32	0.43
1:G:163:VAL:HG13	1:G:165:ILE:HD11	2.00	0.43
1:G:192:ILE:HD12	1:G:253:GLU:CB	2.48	0.43
1:H:16:LEU:HD11	2:H:401:ADP:H5'2	2.01	0.43
1:H:52:SER:O	1:H:53:TYR:CD1	2.71	0.43
1:H:312:ARG:HA	1:H:315:LYS:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:HIS:NE2	1:E:267:ILE:O	2.51	0.43
1:D:280:ASN:OD1	1:D:281:SER:N	2.51	0.43
1:D:361:GLU:H	1:D:361:GLU:HG3	1.41	0.43
1:E:88:HIS:O	1:E:91:TYR:O	2.36	0.43
1:E:213:LYS:O	1:E:217:CYS:HB3	2.18	0.43
1:F:238:LYS:HZ2	1:F:254:ARG:NH2	2.13	0.43
1:F:263:GLN:O	1:F:263:GLN:CG	2.66	0.43
1:F:275:HIS:CD2	1:F:275:HIS:H	2.35	0.43
1:G:105:LEU:CD2	1:G:132:MET:HB2	2.42	0.43
1:G:277:THR:HA	1:G:280:ASN:HD22	1.84	0.43
1:G:295:ALA:HB1	1:G:328:LYS:NZ	2.33	0.43
1:H:142:LEU:HD21	1:H:165:ILE:HB	2.01	0.43
1:H:369:ILE:HG13	1:H:372:ARG:HH22	1.84	0.43
1:D:332:PRO:HA	1:D:333:PRO:HD3	1.89	0.43
1:E:73:HIS:HA	1:E:158:GLY:O	2.18	0.43
1:E:249:THR:O	1:E:249:THR:HG23	2.18	0.43
1:E:267:ILE:CG2	1:E:268:GLY:N	2.81	0.43
1:F:136:ILE:HD12	1:F:139:VAL:CG2	2.39	0.43
1:F:142:LEU:HD21	1:F:165:ILE:HB	2.00	0.43
1:F:196:ARG:NH2	1:F:251:GLY:HA3	2.25	0.43
1:F:289:ILE:HD13	1:F:289:ILE:C	2.38	0.43
1:G:312:ARG:HA	1:G:315:LYS:HE3	2.01	0.43
1:G:370:VAL:HG13	1:G:371:HIS:N	2.33	0.43
1:H:76:ILE:CG2	1:H:79:TRP:H	2.32	0.43
1:H:78:ASN:HD22	1:H:81:ASP:CG	2.21	0.43
1:H:222:ASP:CG	1:H:225:ASN:HB3	2.39	0.43
1:D:138:ALA:CB	1:D:163:VAL:HG11	2.49	0.43
1:E:329:ILE:O	1:E:330:ILE:C	2.56	0.43
1:E:334:GLU:N	1:E:334:GLU:OE2	2.48	0.43
1:F:242:LEU:HG	1:F:246:GLN:C	2.39	0.43
1:F:287:ILE:CG2	1:F:288:ASP:N	2.81	0.43
1:H:105:LEU:CD2	1:H:132:MET:HB2	2.45	0.43
1:H:136:ILE:HD13	1:H:136:ILE:C	2.39	0.43
1:H:165:ILE:HD12	1:H:165:ILE:N	2.34	0.43
1:D:370:VAL:HG13	1:D:371:HIS:N	2.34	0.43
1:E:64:ILE:CD1	1:E:65:LEU:N	2.72	0.43
1:E:105:LEU:CD2	1:E:132:MET:HB2	2.44	0.43
1:E:113:LYS:HG2	1:E:117:GLU:OE2	2.19	0.43
1:E:347:ALA:HA	1:E:356:TRP:HZ2	1.84	0.43
1:F:257:CYS:SG	1:F:258:PRO:N	2.91	0.43
1:G:22:ALA:O	1:G:23:GLY:C	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:LYS:HG2	1:G:117:GLU:CD	2.39	0.43
1:G:267:ILE:CG2	1:G:268:GLY:N	2.81	0.43
1:G:374:CYS:O	1:G:375:PHE:CB	2.67	0.43
1:H:267:ILE:CG2	1:H:268:GLY:N	2.82	0.43
1:D:71:ILE:HD12	1:D:76:ILE:CG1	2.41	0.43
1:D:295:ALA:HB1	1:D:328:LYS:NZ	2.34	0.43
1:E:146:GLY:O	1:E:147:ARG:HB2	2.19	0.43
1:E:238:LYS:CD	1:E:239:SER:H	2.31	0.43
1:F:5:THR:OG1	1:F:101:HIS:HA	2.18	0.43
1:F:53:TYR:C	1:F:54:VAL:HG22	2.38	0.43
1:D:120:THR:O	1:D:124:PHE:HB2	2.19	0.43
1:D:121:GLN:HA	1:D:125:GLU:HG2	2.01	0.43
1:E:279:TYR:O	1:E:282:ILE:HG22	2.19	0.43
1:E:325:MET:CE	1:E:326:LYS:H	2.31	0.43
1:F:138:ALA:CB	1:F:163:VAL:CG1	2.97	0.43
1:F:192:ILE:HD12	1:F:253:GLU:CB	2.48	0.43
1:G:146:GLY:O	1:G:147:ARG:HB2	2.19	0.43
1:D:174:ALA:CB	1:D:281:SER:HA	2.49	0.42
1:E:11:ASP:HB2	1:E:18:LYS:HB2	2.00	0.42
1:E:16:LEU:HD11	2:E:401:ADP:H5'2	2.01	0.42
1:E:160:THR:OG1	1:E:178:LEU:HD13	2.19	0.42
1:E:273:GLY:N	1:E:277:THR:HG23	2.20	0.42
1:F:22:ALA:O	1:F:23:GLY:C	2.57	0.42
1:F:44:MET:HE2	1:F:47:MET:HG2	2.00	0.42
1:F:105:LEU:CD2	1:F:132:MET:HB2	2.44	0.42
1:F:172:PRO:HA	1:F:175:ILE:CD1	2.49	0.42
1:G:64:ILE:H	1:G:64:ILE:HG13	1.53	0.42
1:G:275:HIS:CD2	1:G:275:HIS:H	2.37	0.42
1:H:14:SER:O	1:H:71:ILE:HG23	2.19	0.42
1:H:75:ILE:HG12	1:H:111:ASN:OD1	2.18	0.42
1:D:149:THR:HG23	1:D:166:TYR:HA	2.01	0.42
1:D:242:LEU:HG	1:D:246:GLN:C	2.39	0.42
1:E:22:ALA:O	1:E:23:GLY:C	2.57	0.42
1:E:287:ILE:CG2	1:E:288:ASP:N	2.82	0.42
1:E:289:ILE:C	1:E:289:ILE:HD13	2.40	0.42
1:G:121:GLN:HG3	1:G:362:TYR:OH	2.19	0.42
1:H:6:THR:O	1:H:102:PRO:HD2	2.20	0.42
1:D:61:LYS:CB	1:D:64:ILE:HD11	2.49	0.42
1:E:11:ASP:O	1:E:106:THR:HB	2.19	0.42
1:F:176:MET:HE1	1:F:277:THR:CB	2.41	0.42
1:F:200:PHE:HA	1:F:205:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:VAL:HG23	1:F:340:TRP:H	1.82	0.42
1:F:372:ARG:O	1:F:373:LYS:CB	2.65	0.42
1:G:238:LYS:HZ3	1:G:254:ARG:HH22	1.64	0.42
1:H:136:ILE:HD12	1:H:139:VAL:CG2	2.41	0.42
1:H:222:ASP:OD2	1:H:225:ASN:HB3	2.18	0.42
1:D:139:VAL:HG11	1:F:43:VAL:HG21	2.01	0.42
1:E:14:SER:O	1:E:71:ILE:HG23	2.19	0.42
1:E:206:ARG:HA	1:E:209:VAL:HG12	2.02	0.42
1:F:44:MET:HE3	1:F:45:VAL:H	1.83	0.42
1:F:240:TYR:CZ	1:F:241:GLU:O	2.72	0.42
1:F:300:SER:HA	1:F:335:ARG:HB2	2.02	0.42
1:G:154:ASP:CG	1:G:154:ASP:O	2.58	0.42
1:G:200:PHE:HA	1:G:205:GLU:OE1	2.19	0.42
1:G:325:MET:CE	1:G:326:LYS:H	2.32	0.42
1:H:209:VAL:C	1:H:212:ILE:HG12	2.40	0.42
1:D:120:THR:O	1:D:124:PHE:CB	2.67	0.42
1:D:138:ALA:CB	1:D:163:VAL:CG1	2.98	0.42
1:D:213:LYS:O	1:D:217:CYS:HB3	2.20	0.42
1:E:236:LEU:O	1:E:254:ARG:NH1	2.49	0.42
1:E:238:LYS:HD3	1:E:239:SER:O	2.19	0.42
1:E:323:SER:C	1:E:324:THR:HG23	2.39	0.42
1:E:370:VAL:HG13	1:E:371:HIS:N	2.35	0.42
1:G:136:ILE:HD12	1:G:139:VAL:CG2	2.40	0.42
1:G:263:GLN:O	1:G:265:SER:N	2.52	0.42
1:G:346:LEU:HD11	1:G:355:MET:HE1	2.02	0.42
1:D:37:ARG:HB3	1:D:38:PRO:HD2	2.01	0.42
1:D:62:ARG:NE	1:D:208:ILE:HD11	2.35	0.42
1:D:238:LYS:HE3	1:D:238:LYS:HB2	1.86	0.42
1:E:136:ILE:HD13	1:E:139:VAL:H	1.84	0.42
1:F:11:ASP:HB3	1:F:18:LYS:H	1.84	0.42
1:F:102:PRO:CB	1:F:131:ALA:HB3	2.45	0.42
1:F:111:ASN:CG	1:F:112:PRO:CD	2.88	0.42
1:F:222:ASP:CG	1:F:225:ASN:HB3	2.40	0.42
1:F:224:GLU:C	1:F:224:GLU:CD	2.78	0.42
1:H:129:VAL:HG21	1:H:132:MET:CG	2.39	0.42
1:D:95:ARG:CZ	1:D:95:ARG:HB2	2.50	0.42
1:D:105:LEU:CD2	1:D:132:MET:HB2	2.45	0.42
1:D:209:VAL:C	1:D:212:ILE:HG12	2.39	0.42
1:D:230:ALA:O	1:D:233:SER:O	2.37	0.42
1:E:138:ALA:CB	1:E:163:VAL:CG1	2.97	0.42
1:E:257:CYS:SG	1:E:258:PRO:N	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ASP:O	1:E:296:ASN:HB2	2.20	0.42
1:E:305:MET:O	1:E:306:TYR:O	2.38	0.42
1:H:105:LEU:HD22	1:H:105:LEU:N	2.33	0.42
1:E:22:ALA:HB1	1:E:348:SER:HB2	2.02	0.42
1:E:147:ARG:HH22	1:E:330:ILE:HD12	1.85	0.42
1:E:147:ARG:NH2	1:E:330:ILE:CD1	2.82	0.42
1:E:300:SER:HA	1:E:335:ARG:HB2	2.02	0.42
1:F:16:LEU:HD11	2:F:401:ADP:H5'2	2.02	0.42
1:F:70:PRO:HG3	1:F:85:ILE:CD1	2.49	0.42
1:F:147:ARG:NH2	1:F:330:ILE:CD1	2.82	0.42
1:F:347:ALA:HA	1:F:356:TRP:HZ2	1.85	0.42
1:G:13:GLY:O	1:G:14:SER:OG	2.33	0.42
1:G:111:ASN:CG	1:G:112:PRO:CD	2.88	0.42
1:G:305:MET:O	1:G:306:TYR:O	2.38	0.42
1:G:358:THR:OG1	1:G:359:LYS:N	2.53	0.42
1:H:292:ASP:O	1:H:296:ASN:HB2	2.19	0.42
1:D:214:GLU:HG2	2:D:401:ADP:C2	2.55	0.42
1:E:149:THR:HG23	1:E:166:TYR:HA	2.02	0.42
1:G:147:ARG:HH22	1:G:330:ILE:HD12	1.82	0.42
1:G:280:ASN:OD1	1:G:281:SER:N	2.53	0.42
1:G:332:PRO:HA	1:G:333:PRO:HD3	1.87	0.42
1:H:22:ALA:O	1:H:23:GLY:C	2.58	0.42
1:H:36:GLY:HA3	1:H:66:THR:O	2.20	0.42
1:H:54:VAL:HG11	1:H:88:HIS:HB3	2.02	0.42
1:H:200:PHE:HA	1:H:205:GLU:OE1	2.20	0.42
1:H:286:ASP:OD2	1:H:289:ILE:HG22	2.20	0.42
1:H:361:GLU:O	1:H:364:GLU:HG2	2.20	0.42
1:D:91:TYR:O	1:D:92:ASN:HB2	2.17	0.42
1:D:166:TYR:HD2	1:F:64:ILE:HG21	1.83	0.42
1:E:117:GLU:OE2	1:E:371:HIS:HB2	2.20	0.42
1:E:216:LEU:HD21	1:E:240:TYR:HB2	2.02	0.42
1:E:238:LYS:HZ2	1:E:254:ARG:HH22	1.63	0.42
1:F:43:VAL:CG1	1:F:44:MET:N	2.81	0.42
1:F:61:LYS:HB3	1:F:64:ILE:HD11	2.02	0.42
1:F:318:THR:OG1	1:F:327:ILE:HD11	2.20	0.42
1:G:11:ASP:O	1:G:106:THR:HB	2.20	0.42
1:G:286:ASP:OD2	1:G:289:ILE:HG22	2.20	0.42
1:H:143:TYR:CE2	1:H:346:LEU:HB2	2.54	0.42
1:D:76:ILE:CG2	1:D:79:TRP:H	2.33	0.41
1:D:238:LYS:HZ2	1:D:254:ARG:HH12	1.67	0.41
1:E:70:PRO:HG3	1:E:85:ILE:CD1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASN:OD1	1:E:281:SER:N	2.53	0.41
1:F:188:TYR:O	1:F:192:ILE:HG23	2.20	0.41
1:G:188:TYR:O	1:G:192:ILE:HG23	2.19	0.41
1:G:237:GLU:O	1:G:250:ILE:CD1	2.68	0.41
1:G:374:CYS:C	1:G:375:PHE:HD2	2.24	0.41
1:H:87:HIS:CE1	1:H:91:TYR:HE2	2.37	0.41
1:H:146:GLY:O	1:H:147:ARG:HB2	2.20	0.41
1:H:305:MET:O	1:H:306:TYR:O	2.38	0.41
1:H:329:ILE:N	1:H:329:ILE:CD1	2.72	0.41
1:D:160:THR:OG1	1:D:178:LEU:HD13	2.21	0.41
1:D:229:THR:HG23	1:D:230:ALA:H	1.85	0.41
1:E:129:VAL:HG21	1:E:132:MET:CG	2.39	0.41
1:E:245:GLY:O	1:E:246:GLN:HG3	2.21	0.41
1:F:22:ALA:HB1	1:F:348:SER:CB	2.49	0.41
1:F:76:ILE:CG2	1:F:79:TRP:H	2.34	0.41
1:G:151:ILE:HG12	1:G:164:PRO:HA	2.01	0.41
1:G:216:LEU:HD21	1:G:240:TYR:HB2	2.03	0.41
1:G:309:ILE:HD13	1:G:309:ILE:HA	1.82	0.41
1:H:104:LEU:HD12	1:H:133:TYR:O	2.20	0.41
1:H:121:GLN:HG3	1:H:362:TYR:OH	2.20	0.41
1:H:140:LEU:N	1:H:140:LEU:CD1	2.84	0.41
1:H:325:MET:CE	1:H:326:LYS:H	2.33	0.41
1:D:104:LEU:HD12	1:D:133:TYR:O	2.20	0.41
1:D:249:THR:HG23	1:D:249:THR:O	2.21	0.41
1:E:31:PHE:N	1:E:31:PHE:CD1	2.88	0.41
1:F:18:LYS:CD	1:F:30:VAL:HG13	2.51	0.41
1:G:250:ILE:H	1:G:250:ILE:HD12	1.85	0.41
1:H:358:THR:OG1	1:H:359:LYS:N	2.52	0.41
1:D:200:PHE:O	1:D:201:VAL:HG13	2.21	0.41
1:D:216:LEU:HD21	1:D:240:TYR:HB2	2.02	0.41
1:D:250:ILE:HD12	1:D:250:ILE:H	1.86	0.41
1:D:257:CYS:SG	1:D:258:PRO:N	2.92	0.41
1:E:163:VAL:CG2	1:E:165:ILE:HD11	2.51	0.41
1:E:295:ALA:HB1	1:E:328:LYS:NZ	2.35	0.41
1:F:267:ILE:CG2	1:F:268:GLY:N	2.83	0.41
1:F:352:PHE:CZ	1:H:47:MET:CE	3.03	0.41
1:G:16:LEU:HD11	2:G:401:ADP:H5'2	2.02	0.41
1:G:277:THR:O	1:G:280:ASN:ND2	2.54	0.41
1:H:279:TYR:O	1:H:282:ILE:HG22	2.21	0.41
1:H:309:ILE:HD13	1:H:309:ILE:HA	1.80	0.41
1:H:315:LYS:HB2	1:H:315:LYS:HZ1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TYR:O	1:D:54:VAL:CG2	2.69	0.41
1:D:111:ASN:CG	1:D:112:PRO:CD	2.89	0.41
1:D:124:PHE:CZ	1:D:359:LYS:HA	2.55	0.41
1:D:150:GLY:HA3	1:D:296:ASN:HB3	2.03	0.41
1:D:166:TYR:O	1:D:169:TYR:O	2.39	0.41
1:G:174:ALA:CB	1:G:281:SER:HA	2.50	0.41
1:G:206:ARG:HA	1:G:209:VAL:HG12	2.03	0.41
1:H:43:VAL:CG1	1:H:44:MET:N	2.81	0.41
1:H:79:TRP:HH2	1:H:119:MET:HB2	1.85	0.41
1:D:64:ILE:H	1:D:64:ILE:HG13	1.56	0.41
1:D:279:TYR:O	1:D:282:ILE:HG22	2.21	0.41
1:D:325:MET:SD	1:F:244:ASP:OD2	2.79	0.41
1:E:286:ASP:OD2	1:E:289:ILE:HG22	2.21	0.41
1:G:163:VAL:CG2	1:G:165:ILE:HD11	2.51	0.41
1:G:238:LYS:HZ2	1:G:254:ARG:NH2	2.19	0.41
1:H:18:LYS:CD	1:H:30:VAL:HG13	2.50	0.41
1:H:200:PHE:O	1:H:201:VAL:HG13	2.21	0.41
1:H:280:ASN:OD1	1:H:281:SER:N	2.53	0.41
1:D:146:GLY:O	1:D:147:ARG:HB2	2.21	0.41
1:D:312:ARG:HA	1:D:315:LYS:HE3	2.02	0.41
1:D:323:SER:C	1:D:324:THR:HG23	2.41	0.41
1:E:173:HIS:NE2	1:F:267:ILE:O	2.54	0.41
1:E:242:LEU:HG	1:E:246:GLN:C	2.40	0.41
1:H:346:LEU:HD11	1:H:355:MET:CE	2.51	0.41
1:D:16:LEU:HD11	2:D:401:ADP:H5'2	2.03	0.41
1:D:36:GLY:HA3	1:D:66:THR:O	2.20	0.41
1:D:206:ARG:HA	1:D:209:VAL:HG12	2.03	0.41
1:D:326:LYS:HE3	1:D:327:ILE:N	2.35	0.41
1:E:124:PHE:CZ	1:E:359:LYS:HA	2.56	0.41
1:E:238:LYS:CG	1:E:239:SER:N	2.83	0.41
1:E:352:PHE:HZ	1:G:47:MET:CE	2.34	0.41
1:G:138:ALA:HB1	1:G:163:VAL:HG12	2.03	0.41
1:G:326:LYS:HE3	1:G:327:ILE:N	2.36	0.41
1:H:213:LYS:O	1:H:217:CYS:HB3	2.20	0.41
1:D:286:ASP:OD2	1:D:289:ILE:HG22	2.21	0.41
1:D:374:CYS:C	1:D:375:PHE:HD2	2.24	0.41
1:E:102:PRO:CB	1:E:131:ALA:HB3	2.46	0.41
1:E:242:LEU:CD2	1:E:246:GLN:HB2	2.42	0.41
1:E:323:SER:O	1:E:324:THR:OG1	2.24	0.41
1:E:359:LYS:O	1:E:360:GLN:CB	2.69	0.41
1:F:121:GLN:HG3	1:F:362:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:MET:SD	1:H:244:ASP:OD2	2.79	0.41
1:G:36:GLY:HA3	1:G:66:THR:O	2.21	0.41
1:G:76:ILE:CG2	1:G:79:TRP:H	2.34	0.41
1:G:143:TYR:CE2	1:G:346:LEU:HB2	2.56	0.41
1:G:214:GLU:HG2	2:G:401:ADP:C2	2.56	0.41
1:H:107:GLU:C	1:H:137:GLN:HE21	2.24	0.41
1:H:154:ASP:O	1:H:154:ASP:CG	2.57	0.41
1:H:216:LEU:HD21	1:H:240:TYR:HB2	2.03	0.41
1:D:286:ASP:OD2	1:D:288:ASP:HB3	2.21	0.41
1:D:325:MET:HE2	1:D:326:LYS:H	1.85	0.41
1:E:6:THR:O	1:E:102:PRO:HD2	2.21	0.41
1:E:55:GLY:O	1:E:58:ALA:N	2.54	0.41
1:E:95:ARG:HB2	1:E:95:ARG:CZ	2.50	0.41
1:F:6:THR:O	1:F:102:PRO:HD2	2.21	0.41
1:F:146:GLY:O	1:F:147:ARG:HB2	2.21	0.41
1:F:237:GLU:O	1:F:250:ILE:CD1	2.69	0.41
1:F:325:MET:HE2	1:F:326:LYS:H	1.85	0.41
1:G:8:LEU:N	1:G:102:PRO:O	2.47	0.41
1:G:108:ALA:HA	1:G:109:PRO:HD3	1.93	0.41
1:G:118:LYS:O	1:G:122:ILE:HG12	2.21	0.41
1:H:277:THR:HA	1:H:280:ASN:HD22	1.84	0.41
1:H:286:ASP:CB	1:H:289:ILE:HG22	2.46	0.41
1:D:113:LYS:HG2	1:D:117:GLU:OE2	2.20	0.40
1:D:147:ARG:NH2	1:D:330:ILE:CD1	2.82	0.40
1:D:221:LEU:H	1:D:221:LEU:CD1	2.26	0.40
1:D:238:LYS:CG	1:D:239:SER:N	2.85	0.40
1:E:8:LEU:HD12	1:E:21:PHE:HA	2.02	0.40
1:E:121:GLN:HG3	1:E:362:TYR:OH	2.21	0.40
1:E:188:TYR:O	1:E:192:ILE:HG23	2.20	0.40
1:F:8:LEU:N	1:F:102:PRO:O	2.47	0.40
1:F:29:ALA:HB3	1:F:93:GLU:HB3	2.03	0.40
1:F:37:ARG:HB3	1:F:38:PRO:HD2	2.03	0.40
1:F:222:ASP:OD2	1:F:225:ASN:HB3	2.21	0.40
1:G:43:VAL:CG1	1:G:44:MET:N	2.85	0.40
1:G:160:THR:CG2	1:G:178:LEU:HD13	2.52	0.40
1:G:229:THR:HG23	1:G:230:ALA:H	1.86	0.40
1:H:53:TYR:C	1:H:54:VAL:HG22	2.41	0.40
1:H:118:LYS:O	1:H:122:ILE:HG12	2.20	0.40
1:H:290:ARG:HE	1:H:290:ARG:HB3	1.69	0.40
1:D:66:THR:HA	1:D:203:THR:OG1	2.21	0.40
1:D:169:TYR:CD2	1:F:40:HIS:O	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:GLU:O	1:E:364:GLU:HG2	2.21	0.40
1:F:66:THR:HA	1:F:203:THR:OG1	2.21	0.40
1:F:206:ARG:HA	1:F:209:VAL:HG12	2.03	0.40
1:F:250:ILE:H	1:F:250:ILE:CD1	2.33	0.40
1:G:18:LYS:CD	1:G:30:VAL:HG13	2.52	0.40
1:G:54:VAL:HG11	1:G:88:HIS:HB3	2.03	0.40
1:G:95:ARG:HB2	1:G:95:ARG:CZ	2.51	0.40
1:G:334:GLU:C	1:G:335:ARG:O	2.59	0.40
1:G:369:ILE:CG2	1:G:370:VAL:N	2.83	0.40
1:H:70:PRO:HG3	1:H:85:ILE:CD1	2.51	0.40
1:H:123:MET:HA	1:H:127:PHE:CD2	2.54	0.40
1:H:172:PRO:HA	1:H:175:ILE:CD1	2.50	0.40
1:H:237:GLU:O	1:H:250:ILE:CD1	2.69	0.40
1:H:289:ILE:HD13	1:H:289:ILE:C	2.41	0.40
1:D:11:ASP:O	1:D:106:THR:HB	2.20	0.40
1:D:18:LYS:CD	1:D:30:VAL:HG13	2.51	0.40
1:D:277:THR:O	1:D:280:ASN:ND2	2.55	0.40
1:D:308:GLY:HA2	1:D:311:ASP:OD2	2.22	0.40
1:D:326:LYS:HG3	1:D:328:LYS:NZ	2.37	0.40
1:F:89:THR:O	1:F:94:LEU:HG	2.21	0.40
1:F:110:LEU:HD12	1:F:177:ARG:CG	2.51	0.40
1:F:113:LYS:HG2	1:F:117:GLU:OE2	2.21	0.40
1:F:213:LYS:HD2	1:F:306:TYR:OH	2.22	0.40
1:F:229:THR:HG23	1:F:230:ALA:H	1.87	0.40
1:F:263:GLN:C	1:F:265:SER:N	2.75	0.40
1:F:273:GLY:C	1:F:277:THR:HG23	2.41	0.40
1:H:374:CYS:C	1:H:375:PHE:HD2	2.25	0.40
1:D:31:PHE:N	1:D:31:PHE:CD1	2.90	0.40
1:E:223:PHE:O	1:E:226:GLU:HB2	2.22	0.40
1:E:224:GLU:C	1:E:224:GLU:CD	2.80	0.40
1:E:326:LYS:HG3	1:E:328:LYS:NZ	2.37	0.40
1:F:123:MET:HA	1:F:127:PHE:CD2	2.54	0.40
1:F:286:ASP:OD2	1:F:289:ILE:HG22	2.22	0.40
1:F:329:ILE:N	1:F:329:ILE:CD1	2.76	0.40
1:F:336:LYS:HE2	1:F:337:TYR:CZ	2.55	0.40
1:G:22:ALA:HB1	1:G:348:SER:CB	2.51	0.40
1:H:29:ALA:HB3	1:H:93:GLU:HB3	2.03	0.40
1:D:139:VAL:CG2	1:F:43:VAL:HG11	2.51	0.40
1:D:147:ARG:HH22	1:D:330:ILE:HD12	1.84	0.40
1:E:142:LEU:HD21	1:E:165:ILE:HB	2.02	0.40
1:F:31:PHE:HB2	1:F:56:ASP:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:TRP:HH2	1:F:119:MET:HB2	1.86	0.40
1:F:124:PHE:CZ	1:F:359:LYS:HA	2.56	0.40
1:F:326:LYS:HE3	1:F:327:ILE:N	2.35	0.40
1:F:374:CYS:C	1:F:375:PHE:HD2	2.24	0.40
1:H:55:GLY:O	1:H:58:ALA:N	2.54	0.40
1:H:108:ALA:HA	1:H:109:PRO:HD3	1.93	0.40
1:H:110:LEU:HD11	1:H:175:ILE:CB	2.50	0.40
1:H:124:PHE:CZ	1:H:359:LYS:HA	2.56	0.40
1:H:250:ILE:HD12	1:H:250:ILE:H	1.87	0.40
1:H:257:CYS:SG	1:H:258:PRO:N	2.94	0.40
1:H:353:GLN:N	1:H:353:GLN:NE2	2.70	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	D	373/377 (99%)	326 (87%)	24 (6%)	23 (6%)	1	19
1	E	373/377 (99%)	326 (87%)	24 (6%)	23 (6%)	1	19
1	F	373/377 (99%)	326 (87%)	24 (6%)	23 (6%)	1	19
1	G	373/377 (99%)	327 (88%)	24 (6%)	22 (6%)	1	19
1	H	373/377 (99%)	327 (88%)	24 (6%)	22 (6%)	1	19
All	All	1865/1885 (99%)	1632 (88%)	120 (6%)	113 (6%)	3	19

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	ASN
1	D	144	ALA
1	D	223	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	SER
1	D	351	THR
1	E	92	ASN
1	E	144	ALA
1	E	223	PHE
1	E	235	SER
1	E	351	THR
1	F	92	ASN
1	F	144	ALA
1	F	223	PHE
1	F	235	SER
1	F	251	GLY
1	F	351	THR
1	G	92	ASN
1	G	144	ALA
1	G	223	PHE
1	G	235	SER
1	G	351	THR
1	H	92	ASN
1	H	144	ALA
1	H	223	PHE
1	H	235	SER
1	H	351	THR
1	D	22	ALA
1	D	23	GLY
1	D	35	VAL
1	D	201	VAL
1	D	211	ASP
1	D	251	GLY
1	D	303	THR
1	D	335	ARG
1	D	350	SER
1	E	14	SER
1	E	22	ALA
1	E	23	GLY
1	E	35	VAL
1	E	201	VAL
1	E	211	ASP
1	E	251	GLY
1	E	303	THR
1	E	350	SER
1	F	14	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	22	ALA
1	F	23	GLY
1	F	35	VAL
1	F	201	VAL
1	F	211	ASP
1	F	303	THR
1	F	335	ARG
1	F	350	SER
1	G	22	ALA
1	G	23	GLY
1	G	35	VAL
1	G	201	VAL
1	G	211	ASP
1	G	251	GLY
1	G	303	THR
1	G	350	SER
1	H	22	ALA
1	H	23	GLY
1	H	35	VAL
1	H	201	VAL
1	H	211	ASP
1	H	251	GLY
1	H	303	THR
1	H	335	ARG
1	H	350	SER
1	D	14	SER
1	D	79	TRP
1	E	79	TRP
1	E	335	ARG
1	F	79	TRP
1	G	14	SER
1	G	335	ARG
1	H	14	SER
1	H	79	TRP
1	H	360	GLN
1	D	360	GLN
1	F	26	ALA
1	F	360	GLN
1	G	26	ALA
1	G	79	TRP
1	G	360	GLN
1	D	26	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	264	PRO
1	E	26	ALA
1	E	217	CYS
1	E	243	PRO
1	E	264	PRO
1	E	360	GLN
1	F	264	PRO
1	G	243	PRO
1	G	264	PRO
1	H	26	ALA
1	H	243	PRO
1	H	264	PRO
1	D	243	PRO
1	D	306	TYR
1	E	306	TYR
1	F	306	TYR
1	G	306	TYR
1	H	306	TYR
1	G	330	ILE
1	H	330	ILE
1	D	158	GLY
1	D	330	ILE
1	F	158	GLY
1	F	330	ILE
1	E	330	ILE
1	F	243	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	D	318/320 (99%)	275 (86%)	43 (14%)	4	19
1	E	318/320 (99%)	275 (86%)	43 (14%)	4	19
1	F	318/320 (99%)	274 (86%)	44 (14%)	3	19
1	G	318/320 (99%)	274 (86%)	44 (14%)	3	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	318/320 (99%)	275 (86%)	43 (14%)	4	19
All	All	1590/1600 (99%)	1373 (86%)	217 (14%)	7	19

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	ASP
1	D	10	CYS
1	D	31	PHE
1	D	45	VAL
1	D	49	GLN
1	D	66	THR
1	D	79	TRP
1	D	105	LEU
1	D	106	THR
1	D	118	LYS
1	D	134	VAL
1	D	136	ILE
1	D	147	ARG
1	D	160	THR
1	D	171	LEU
1	D	176	MET
1	D	178	LEU
1	D	201	VAL
1	D	202	THR
1	D	216	LEU
1	D	217	CYS
1	D	227	MET
1	D	236	LEU
1	D	238	LYS
1	D	242	LEU
1	D	250	ILE
1	D	253	GLU
1	D	257	CYS
1	D	265	SER
1	D	267	ILE
1	D	289	ILE
1	D	306	TYR
1	D	313	MET
1	D	320	LEU
1	D	326	LYS
1	D	327	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	329	ILE
1	D	336	LYS
1	D	349	LEU
1	D	351	THR
1	D	361	GLU
1	D	371	HIS
1	D	373	LYS
1	E	3	ASP
1	E	10	CYS
1	E	31	PHE
1	E	45	VAL
1	E	49	GLN
1	E	66	THR
1	E	79	TRP
1	E	105	LEU
1	E	106	THR
1	E	118	LYS
1	E	134	VAL
1	E	136	ILE
1	E	147	ARG
1	E	160	THR
1	E	171	LEU
1	E	176	MET
1	E	178	LEU
1	E	201	VAL
1	E	202	THR
1	E	216	LEU
1	E	217	CYS
1	E	227	MET
1	E	236	LEU
1	E	238	LYS
1	E	242	LEU
1	E	250	ILE
1	E	253	GLU
1	E	257	CYS
1	E	265	SER
1	E	267	ILE
1	E	289	ILE
1	E	306	TYR
1	E	313	MET
1	E	320	LEU
1	E	326	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	327	ILE
1	E	329	ILE
1	E	336	LYS
1	E	349	LEU
1	E	351	THR
1	E	361	GLU
1	E	371	HIS
1	E	373	LYS
1	F	3	ASP
1	F	10	CYS
1	F	31	PHE
1	F	45	VAL
1	F	49	GLN
1	F	66	THR
1	F	79	TRP
1	F	105	LEU
1	F	106	THR
1	F	118	LYS
1	F	134	VAL
1	F	136	ILE
1	F	147	ARG
1	F	160	THR
1	F	171	LEU
1	F	176	MET
1	F	178	LEU
1	F	201	VAL
1	F	202	THR
1	F	216	LEU
1	F	217	CYS
1	F	227	MET
1	F	236	LEU
1	F	238	LYS
1	F	242	LEU
1	F	250	ILE
1	F	253	GLU
1	F	257	CYS
1	F	259	GLU
1	F	265	SER
1	F	267	ILE
1	F	289	ILE
1	F	306	TYR
1	F	313	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	320	LEU
1	F	326	LYS
1	F	327	ILE
1	F	329	ILE
1	F	336	LYS
1	F	349	LEU
1	F	351	THR
1	F	361	GLU
1	F	371	HIS
1	F	373	LYS
1	G	3	ASP
1	G	5	THR
1	G	10	CYS
1	G	31	PHE
1	G	45	VAL
1	G	49	GLN
1	G	66	THR
1	G	79	TRP
1	G	105	LEU
1	G	106	THR
1	G	118	LYS
1	G	134	VAL
1	G	136	ILE
1	G	147	ARG
1	G	160	THR
1	G	171	LEU
1	G	176	MET
1	G	178	LEU
1	G	201	VAL
1	G	202	THR
1	G	216	LEU
1	G	217	CYS
1	G	227	MET
1	G	236	LEU
1	G	238	LYS
1	G	242	LEU
1	G	250	ILE
1	G	253	GLU
1	G	257	CYS
1	G	265	SER
1	G	267	ILE
1	G	289	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	306	TYR
1	G	313	MET
1	G	320	LEU
1	G	326	LYS
1	G	327	ILE
1	G	329	ILE
1	G	336	LYS
1	G	349	LEU
1	G	351	THR
1	G	361	GLU
1	G	371	HIS
1	G	373	LYS
1	H	3	ASP
1	H	10	CYS
1	H	31	PHE
1	H	45	VAL
1	H	49	GLN
1	H	66	THR
1	H	79	TRP
1	H	105	LEU
1	H	106	THR
1	H	118	LYS
1	H	134	VAL
1	H	136	ILE
1	H	147	ARG
1	H	160	THR
1	H	171	LEU
1	H	176	MET
1	H	178	LEU
1	H	201	VAL
1	H	202	THR
1	H	216	LEU
1	H	217	CYS
1	H	227	MET
1	H	236	LEU
1	H	238	LYS
1	H	242	LEU
1	H	250	ILE
1	H	253	GLU
1	H	257	CYS
1	H	265	SER
1	H	267	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	289	ILE
1	H	306	TYR
1	H	313	MET
1	H	320	LEU
1	H	326	LYS
1	H	327	ILE
1	H	329	ILE
1	H	336	LYS
1	H	349	LEU
1	H	351	THR
1	H	361	GLU
1	H	371	HIS
1	H	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	12	ASN
1	D	59	GLN
1	D	78	ASN
1	D	87	HIS
1	D	92	ASN
1	D	115	ASN
1	D	137	GLN
1	D	162	ASN
1	D	263	GLN
1	D	275	HIS
1	D	296	ASN
1	D	353	GLN
1	E	12	ASN
1	E	59	GLN
1	E	78	ASN
1	E	87	HIS
1	E	92	ASN
1	E	115	ASN
1	E	137	GLN
1	E	162	ASN
1	E	263	GLN
1	E	275	HIS
1	E	296	ASN
1	E	353	GLN
1	F	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	59	GLN
1	F	78	ASN
1	F	87	HIS
1	F	92	ASN
1	F	115	ASN
1	F	137	GLN
1	F	162	ASN
1	F	263	GLN
1	F	275	HIS
1	F	296	ASN
1	F	353	GLN
1	F	354	GLN
1	G	12	ASN
1	G	59	GLN
1	G	78	ASN
1	G	87	HIS
1	G	92	ASN
1	G	115	ASN
1	G	137	GLN
1	G	162	ASN
1	G	263	GLN
1	G	275	HIS
1	G	296	ASN
1	G	297	ASN
1	G	353	GLN
1	H	12	ASN
1	H	59	GLN
1	H	78	ASN
1	H	87	HIS
1	H	92	ASN
1	H	115	ASN
1	H	137	GLN
1	H	162	ASN
1	H	263	GLN
1	H	275	HIS
1	H	296	ASN
1	H	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	G	401	3	24,29,29	1.57	4 (16%)	29,45,45	1.47	1 (3%)
2	ADP	F	401	3	24,29,29	1.44	5 (20%)	29,45,45	1.61	1 (3%)
2	ADP	H	401	3	24,29,29	1.43	4 (16%)	29,45,45	1.59	1 (3%)
2	ADP	D	401	3	24,29,29	1.41	5 (20%)	29,45,45	1.59	1 (3%)
2	ADP	E	401	3	24,29,29	1.50	5 (20%)	29,45,45	1.54	1 (3%)

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	G	401	3	-	6/12/32/32	0/3/3/3
2	ADP	F	401	3	-	6/12/32/32	0/3/3/3
2	ADP	H	401	3	-	6/12/32/32	0/3/3/3
2	ADP	D	401	3	-	6/12/32/32	0/3/3/3
2	ADP	E	401	3	-	6/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	ADP	C2-N3	3.59	1.37	1.32
2	G	401	ADP	C4-N3	3.55	1.40	1.35
2	H	401	ADP	O4'-C1'	3.24	1.45	1.41
2	E	401	ADP	C2-N3	3.14	1.37	1.32
2	D	401	ADP	C2-N3	3.12	1.37	1.32
2	E	401	ADP	O4'-C1'	3.12	1.45	1.41
2	F	401	ADP	O4'-C1'	3.04	1.45	1.41
2	E	401	ADP	C4-N3	2.91	1.39	1.35
2	G	401	ADP	O4'-C1'	2.89	1.45	1.41
2	H	401	ADP	C2-N3	2.86	1.36	1.32
2	D	401	ADP	O4'-C1'	2.82	1.45	1.41
2	F	401	ADP	C2-N3	2.79	1.36	1.32
2	F	401	ADP	C5-N7	-2.29	1.31	1.39
2	D	401	ADP	C5-N7	-2.25	1.31	1.39
2	H	401	ADP	C4-N3	2.25	1.38	1.35
2	H	401	ADP	C5-N7	-2.24	1.31	1.39
2	E	401	ADP	C5'-C4'	2.24	1.58	1.51
2	F	401	ADP	C5'-C4'	2.19	1.58	1.51
2	G	401	ADP	C5'-C4'	2.17	1.58	1.51
2	F	401	ADP	C4-N3	2.16	1.38	1.35
2	D	401	ADP	C5'-C4'	2.05	1.58	1.51
2	D	401	ADP	C4-N3	2.05	1.38	1.35
2	E	401	ADP	C5-N7	-2.05	1.32	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	ADP	N3-C2-N1	-7.23	117.37	128.68
2	D	401	ADP	N3-C2-N1	-7.12	117.55	128.68
2	H	401	ADP	N3-C2-N1	-7.11	117.57	128.68
2	E	401	ADP	N3-C2-N1	-6.80	118.05	128.68
2	G	401	ADP	N3-C2-N1	-6.19	119.01	128.68

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	ADP	C5'-O5'-PA-O1A
2	D	401	ADP	C5'-O5'-PA-O2A
2	D	401	ADP	C5'-O5'-PA-O3A
2	E	401	ADP	C5'-O5'-PA-O1A
2	E	401	ADP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	401	ADP	C5'-O5'-PA-O3A
2	F	401	ADP	C5'-O5'-PA-O1A
2	F	401	ADP	C5'-O5'-PA-O2A
2	F	401	ADP	C5'-O5'-PA-O3A
2	G	401	ADP	C5'-O5'-PA-O1A
2	G	401	ADP	C5'-O5'-PA-O2A
2	G	401	ADP	C5'-O5'-PA-O3A
2	H	401	ADP	C5'-O5'-PA-O1A
2	H	401	ADP	C5'-O5'-PA-O2A
2	H	401	ADP	C5'-O5'-PA-O3A
2	D	401	ADP	PB-O3A-PA-O1A
2	E	401	ADP	PB-O3A-PA-O1A
2	F	401	ADP	PB-O3A-PA-O1A
2	G	401	ADP	PB-O3A-PA-O1A
2	H	401	ADP	PB-O3A-PA-O1A
2	G	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	C3'-C4'-C5'-O5'
2	D	401	ADP	C3'-C4'-C5'-O5'
2	H	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	C3'-C4'-C5'-O5'
2	G	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	O4'-C4'-C5'-O5'
2	F	401	ADP	O4'-C4'-C5'-O5'
2	H	401	ADP	O4'-C4'-C5'-O5'
2	E	401	ADP	O4'-C4'-C5'-O5'

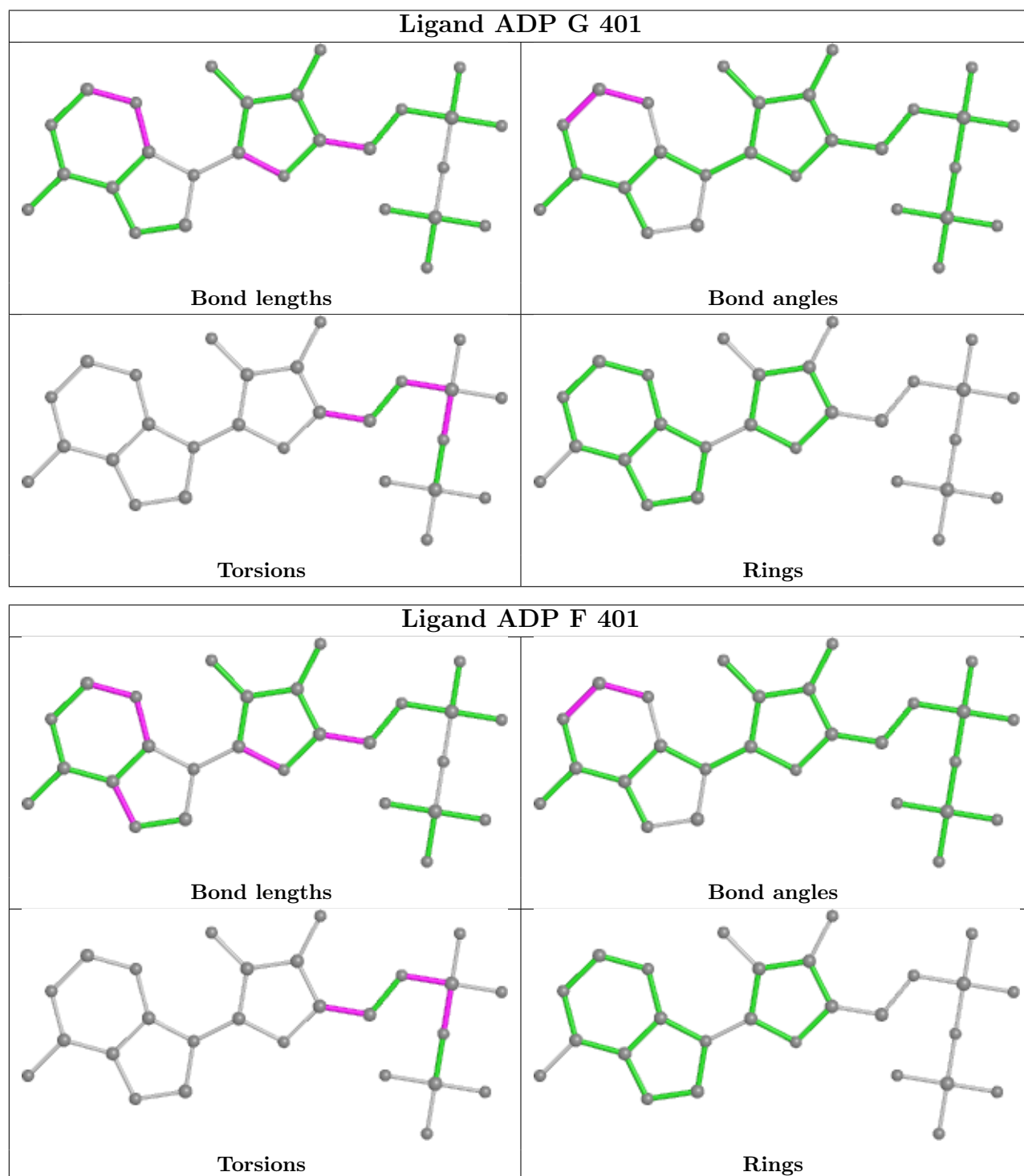
There are no ring outliers.

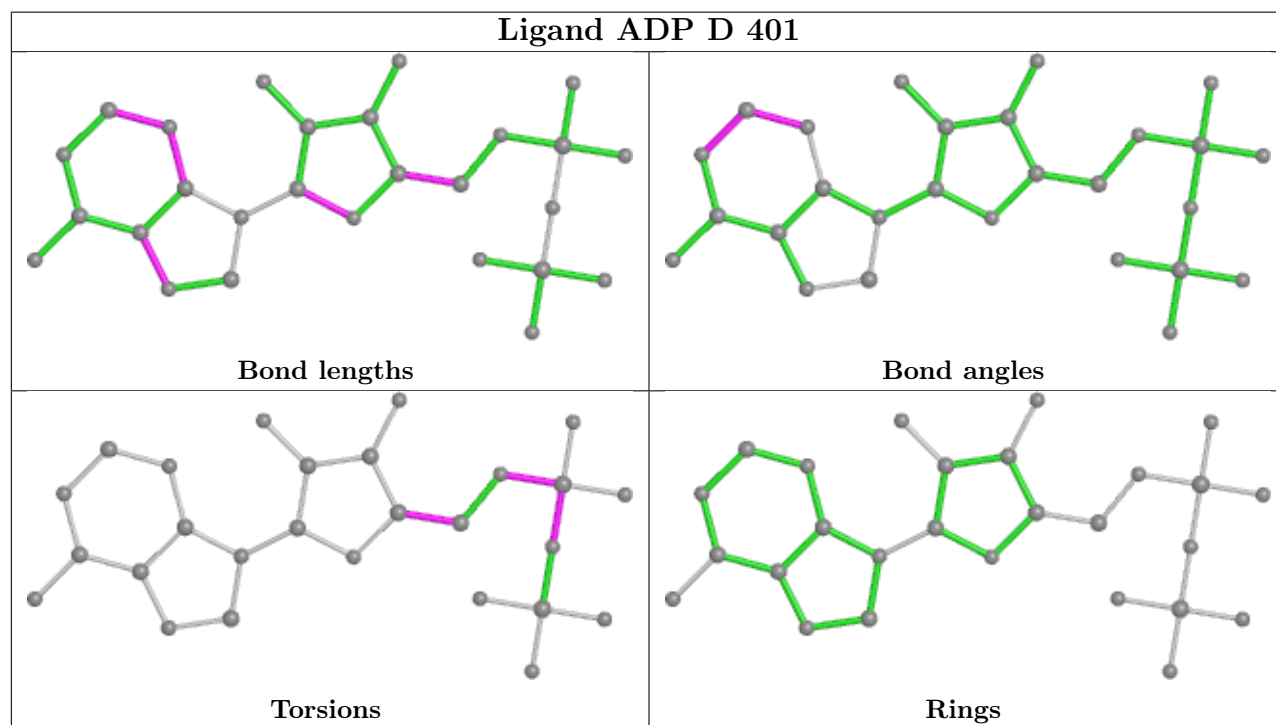
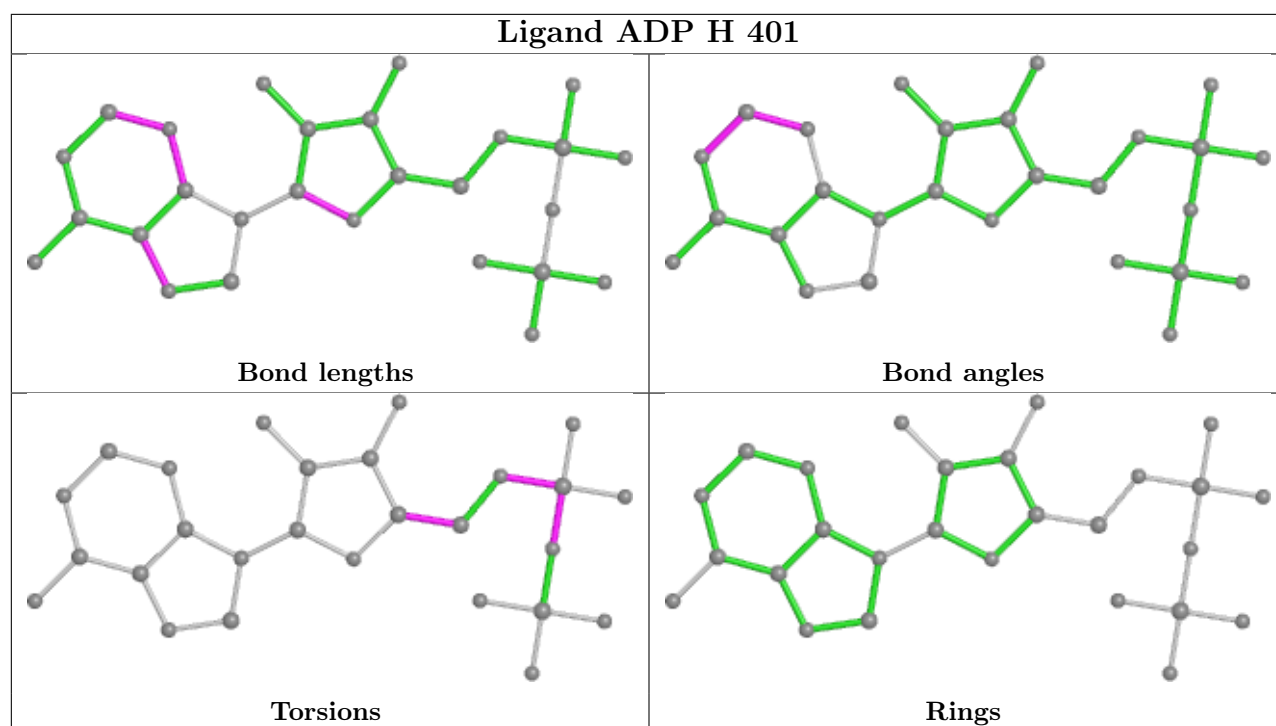
5 monomers are involved in 10 short contacts:

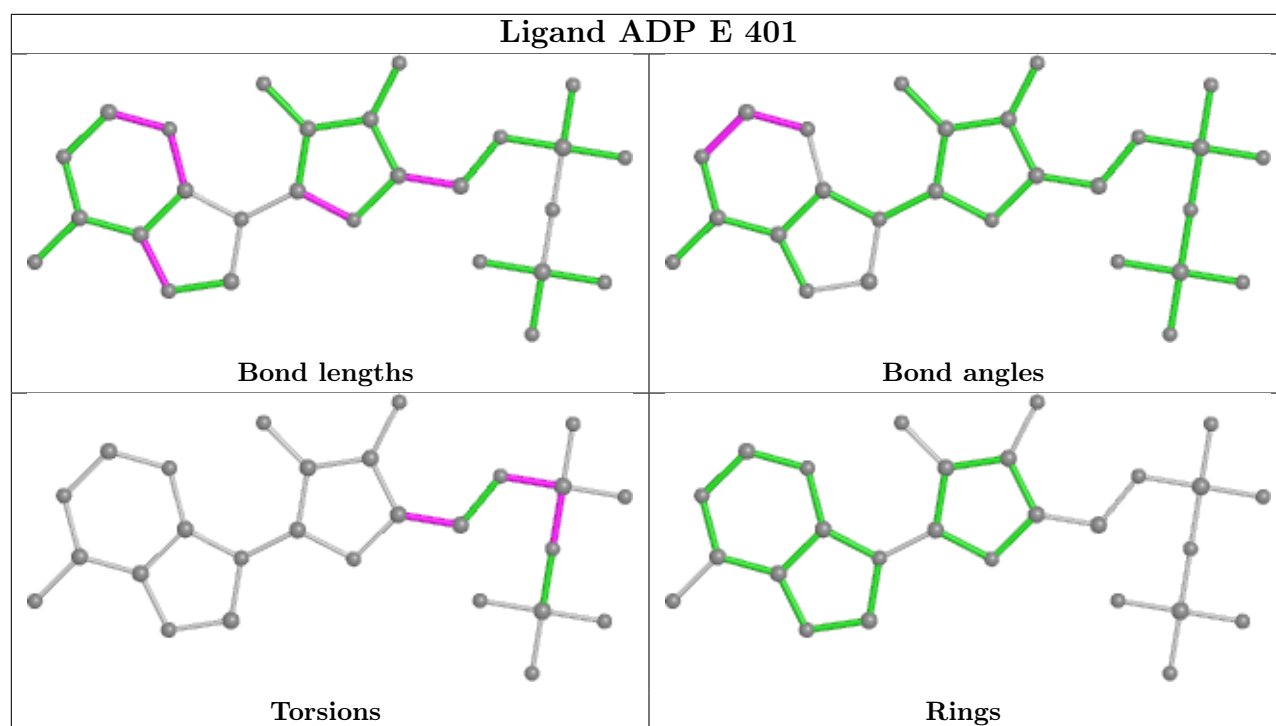
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	ADP	2	0
2	F	401	ADP	2	0
2	H	401	ADP	2	0
2	D	401	ADP	2	0
2	E	401	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

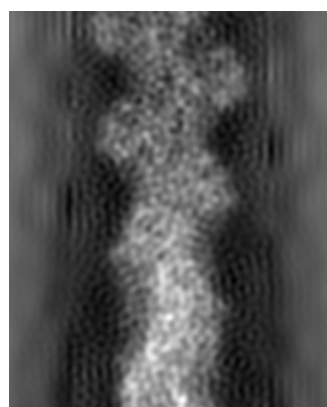
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6179. These allow visual inspection of the internal detail of the map and identification of artifacts.

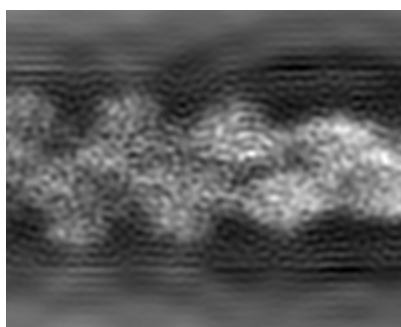
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

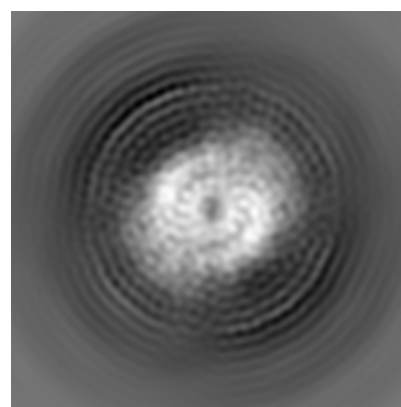
6.1.1 Primary map



X



Y



Z

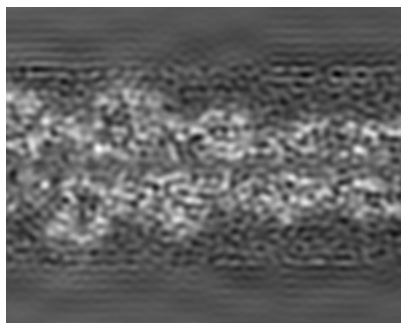
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

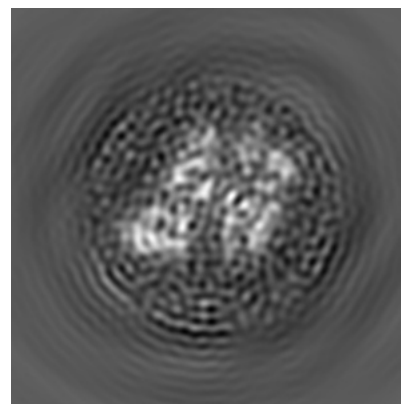
6.2.1 Primary map



X Index: 80



Y Index: 80

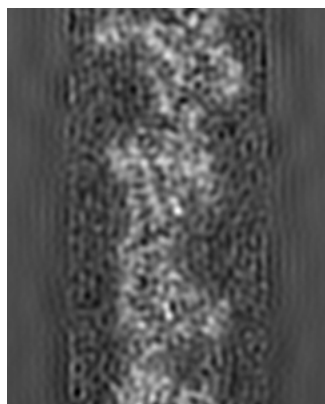


Z Index: 100

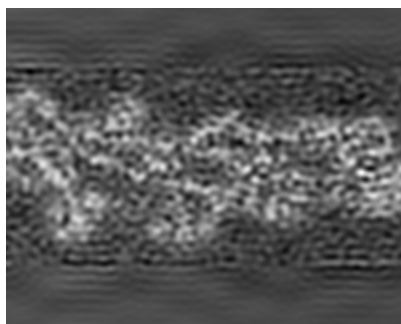
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

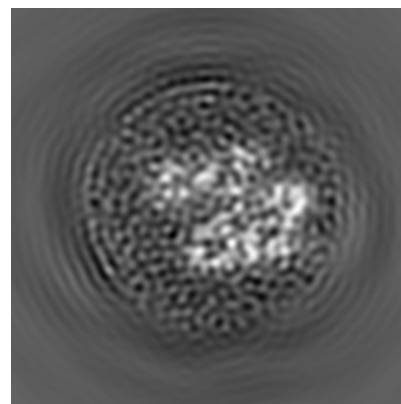
6.3.1 Primary map



X Index: 88



Y Index: 72



Z Index: 1

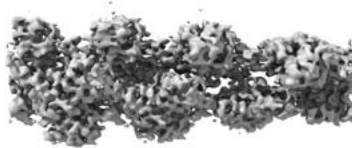
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

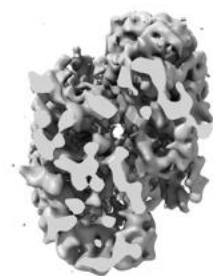
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

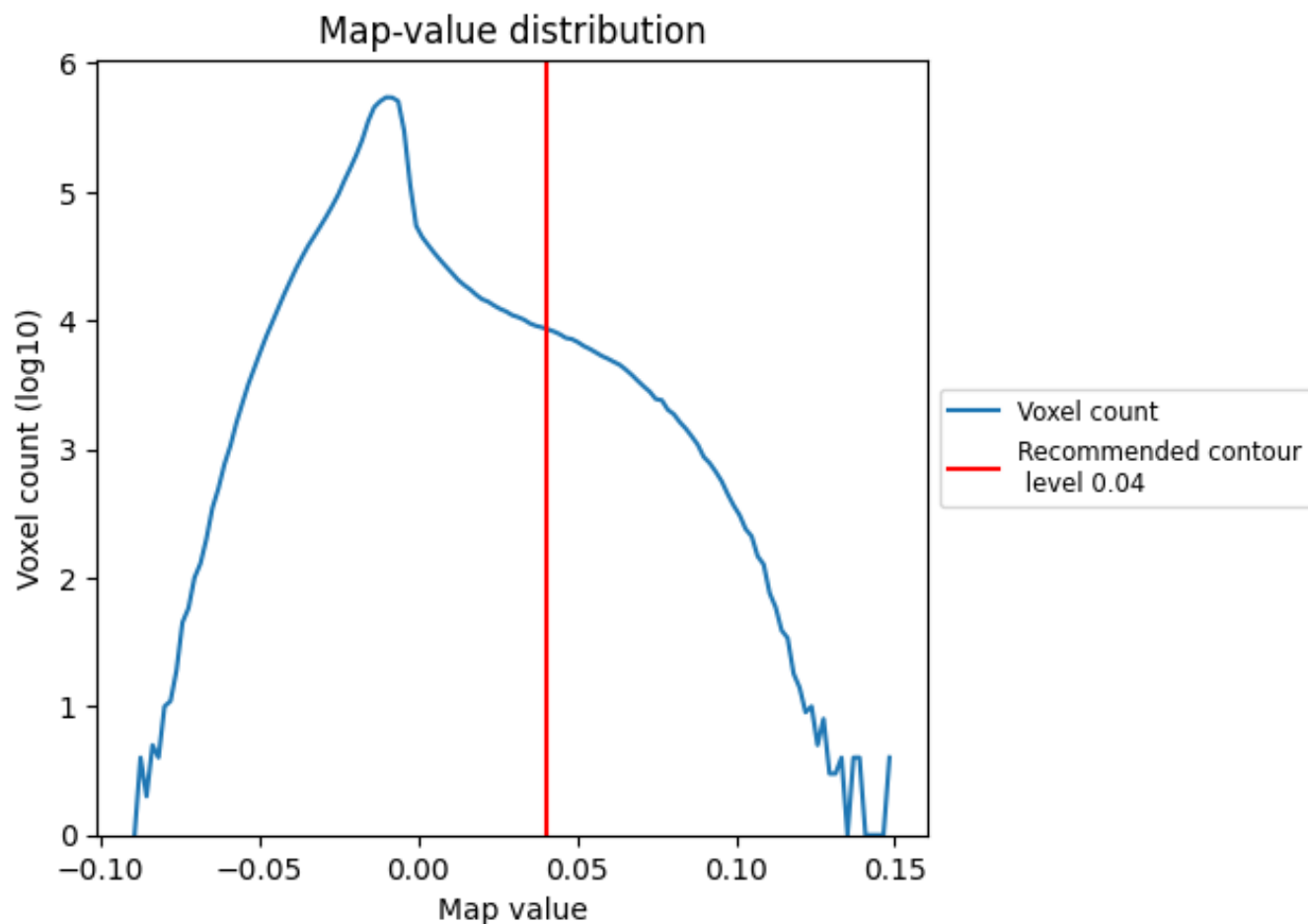
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

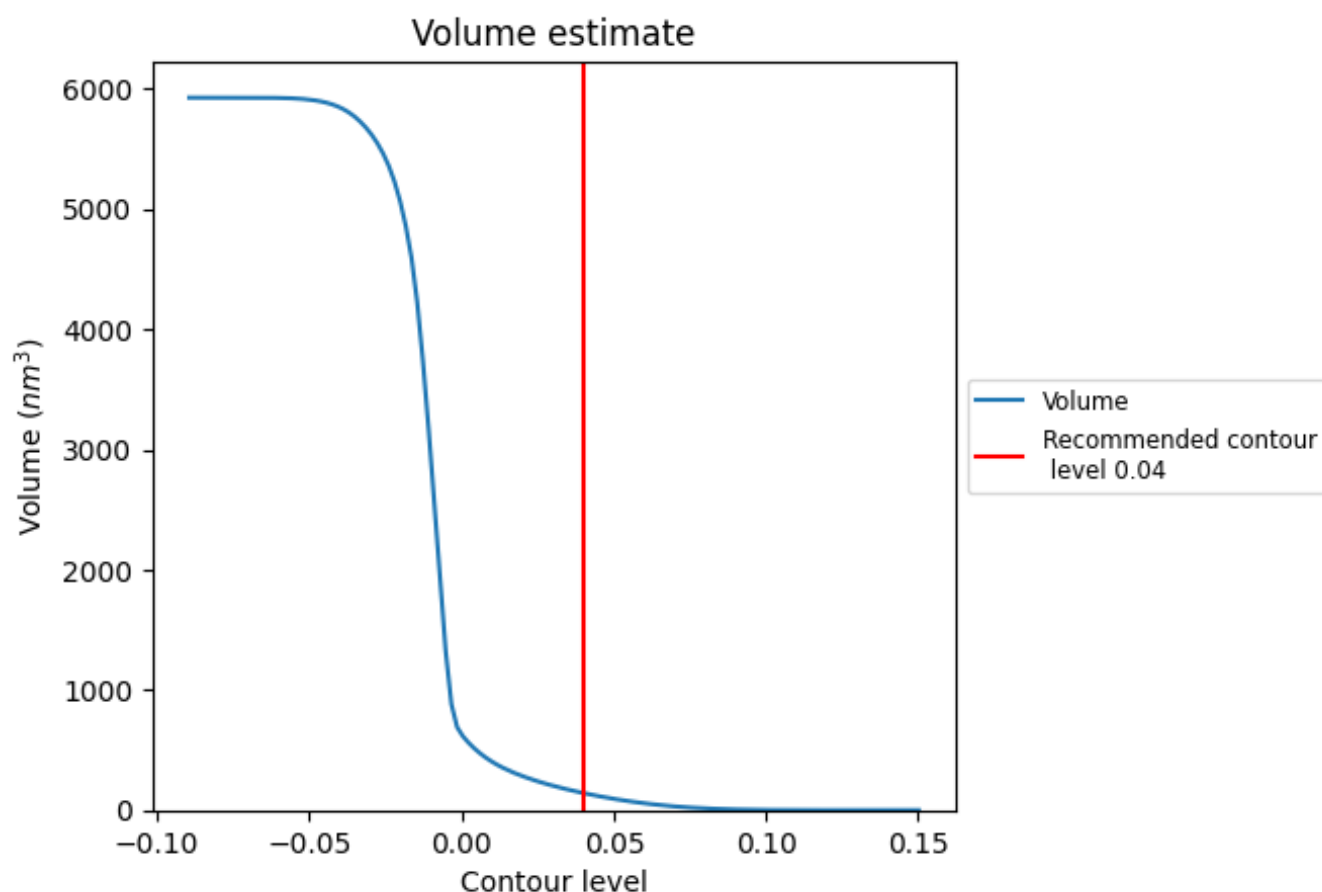
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 129 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

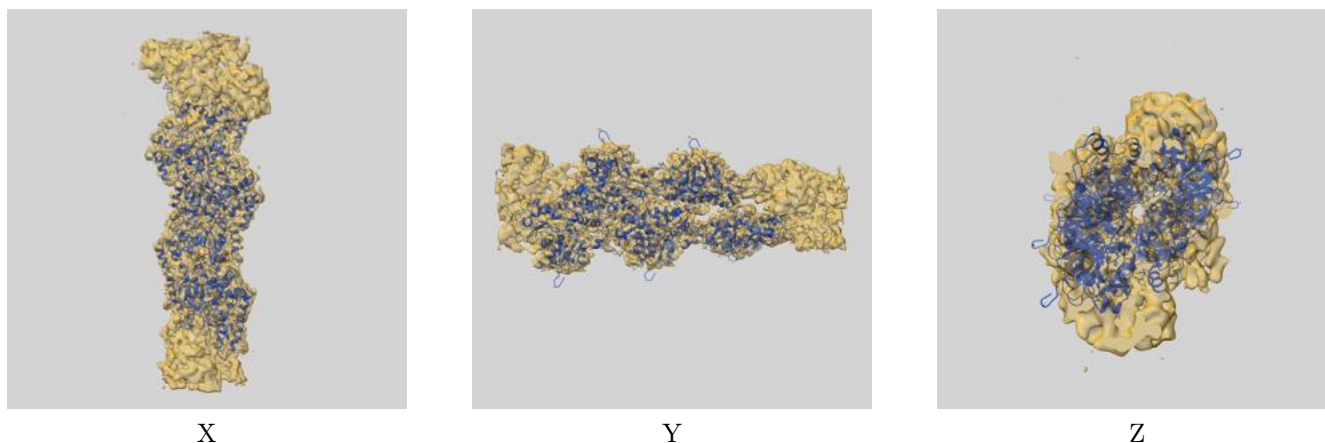
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

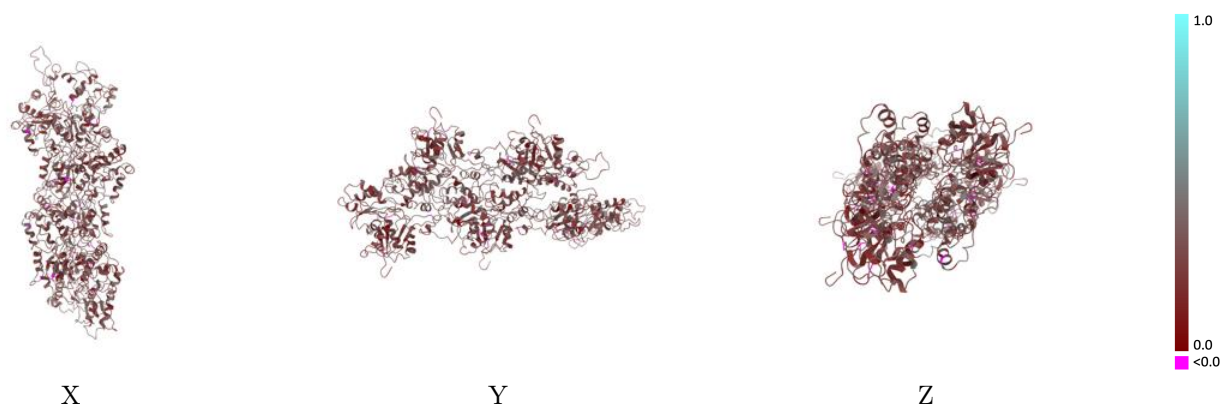
This section contains information regarding the fit between EMDB map EMD-6179 and PDB model 3J8I. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



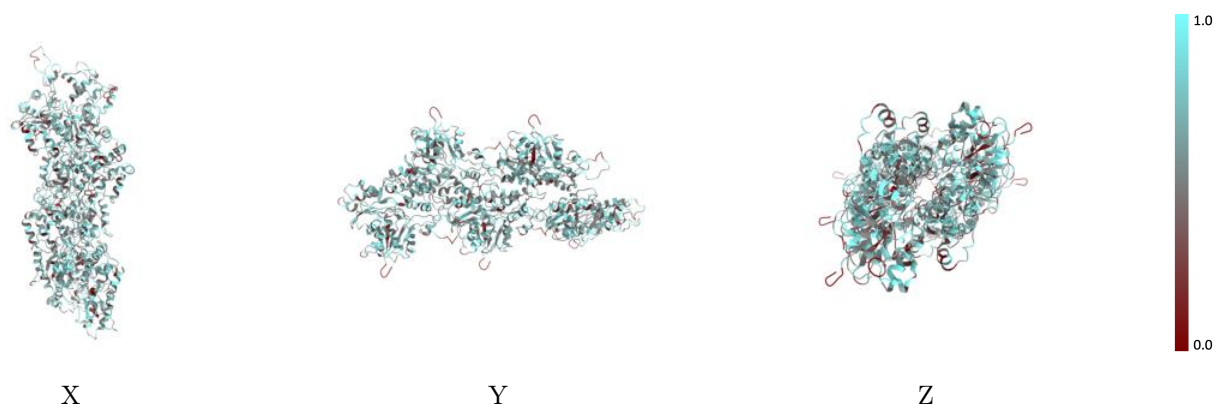
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



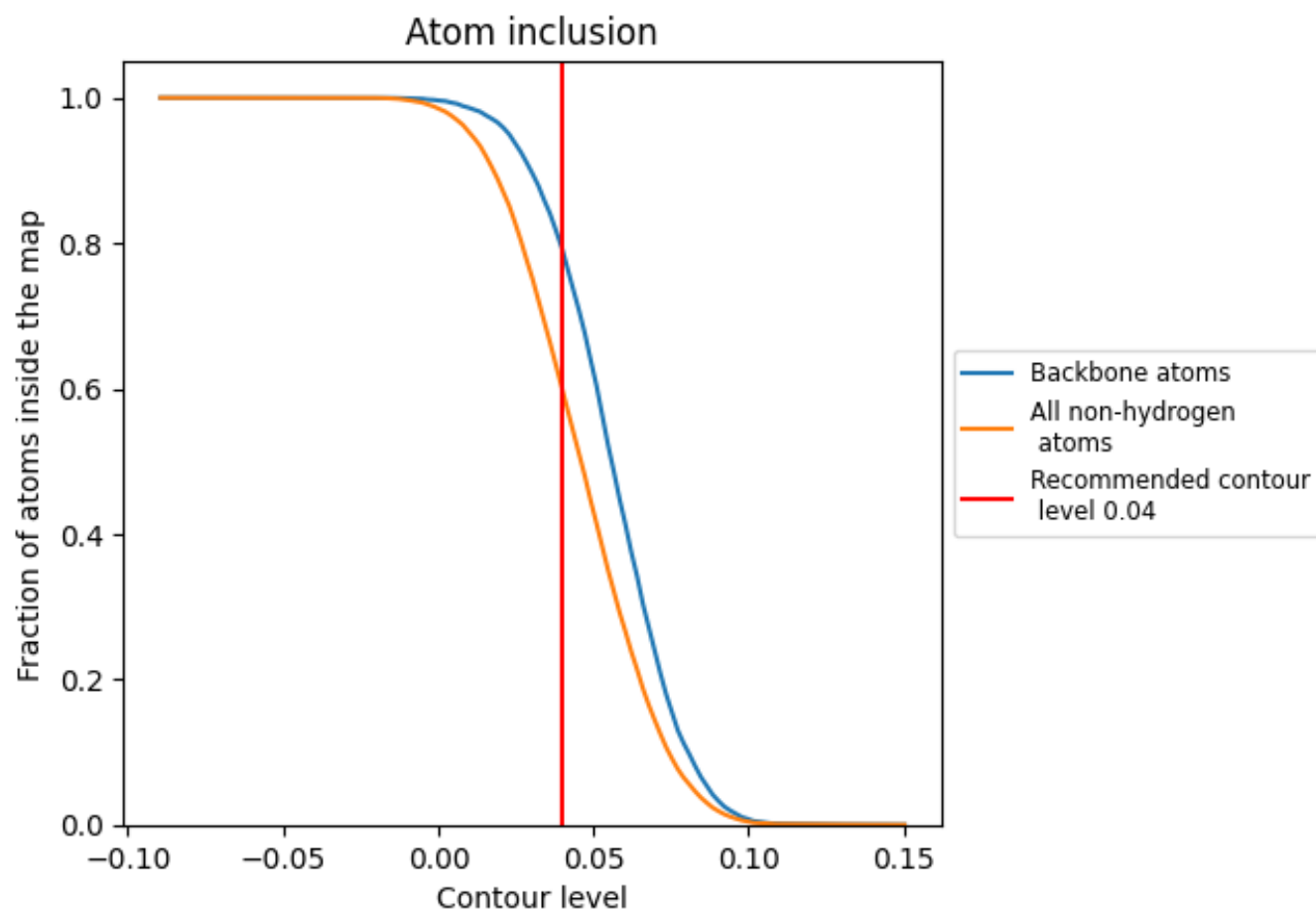
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5980	<div></div> 0.2880
D	<div></div> 0.5923	<div></div> 0.2840
E	<div></div> 0.5978	<div></div> 0.2940
F	<div></div> 0.5954	<div></div> 0.2830
G	<div></div> 0.6071	<div></div> 0.2960
H	<div></div> 0.5975	<div></div> 0.2820

