Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:54 AM EST

PDB ID	:	3J8K
EMDB ID	:	EMD-6181
Title	:	Tilted state of actin, T2
Authors	:	Galkin, V.E.; Orlova, A.; Vos, M.R.; Schroder, G.F.; Egelman, E.H.
Deposited on	:	2014-11-07
Resolution	:	12.00 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:

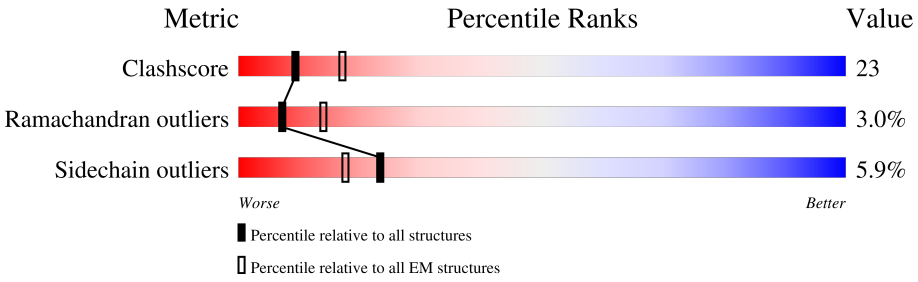
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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 <=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	A	377	95% 58% 37%
1	B	377	52% 63% 33%
1	C	377	45% 60% 36%
1	D	377	42% 51% 43% 5%
1	E	377	44% 55% 41%
1	F	377	43% 54% 40% 5%
1	G	377	44% 57% 38%
1	H	377	44% 55% 40%

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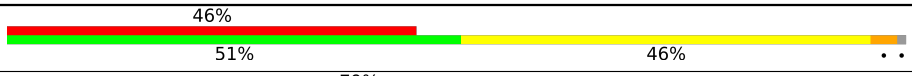
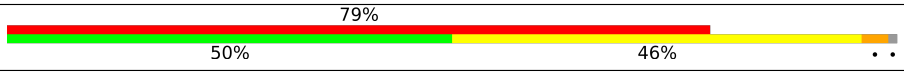
Mol	Chain	Length	Quality of chain
1	I	377	
1	J	377	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 29330 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.

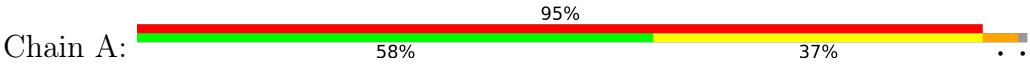
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

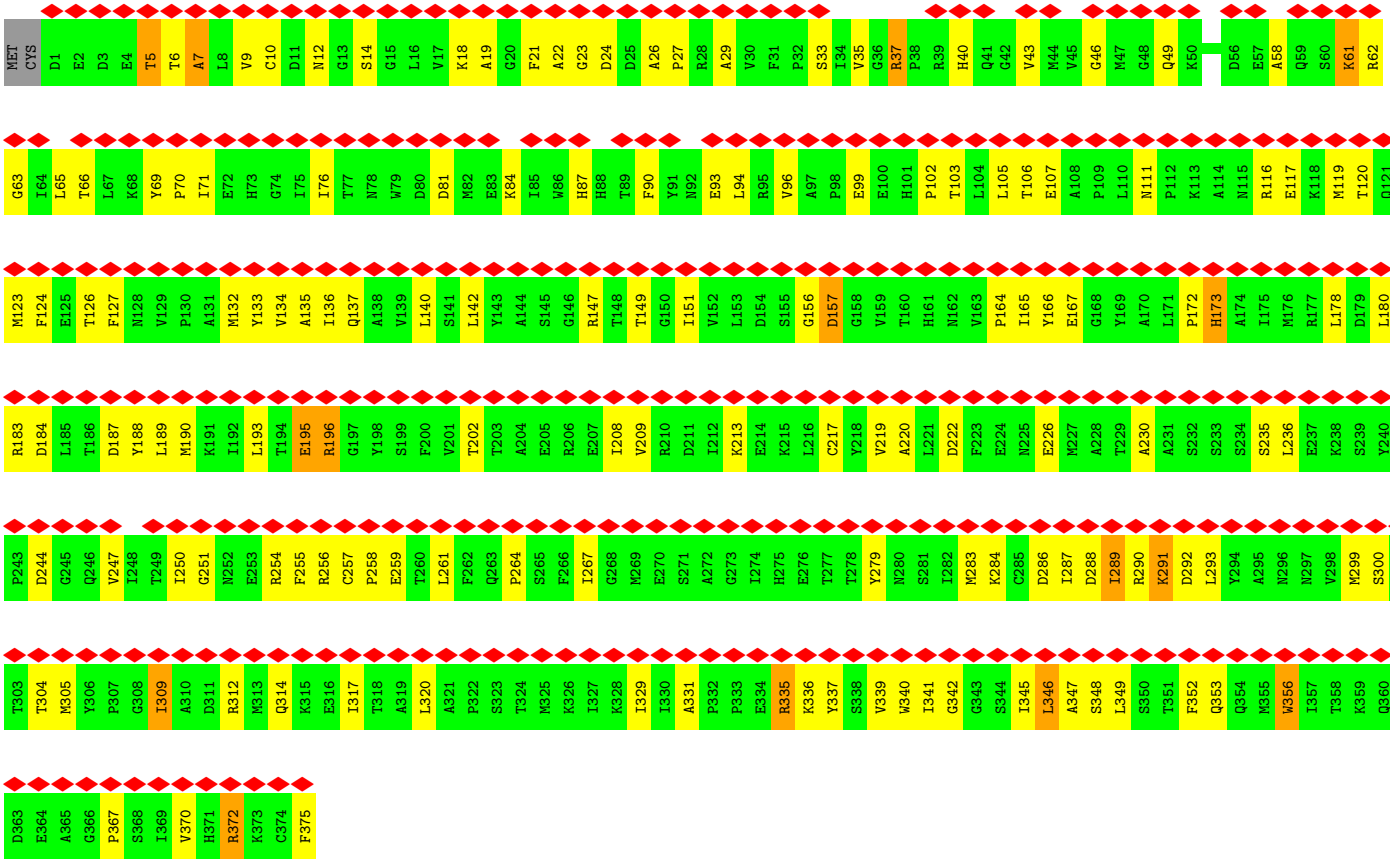
3 Residue-property plots (i)

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

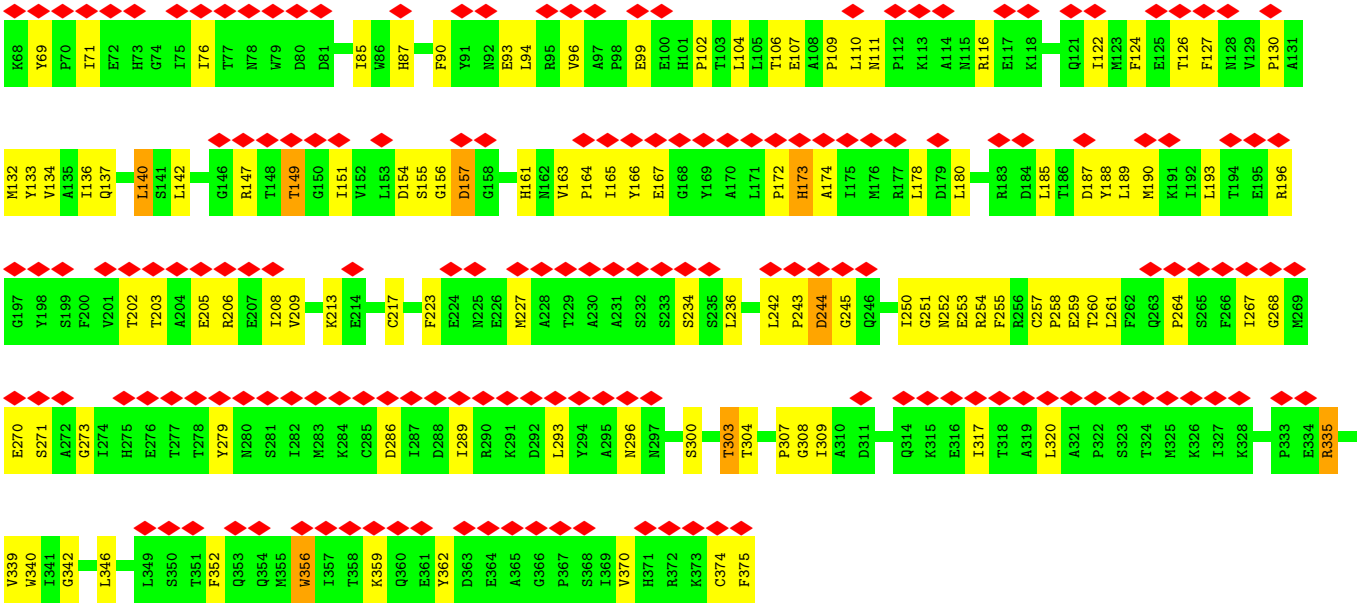
Chain A:





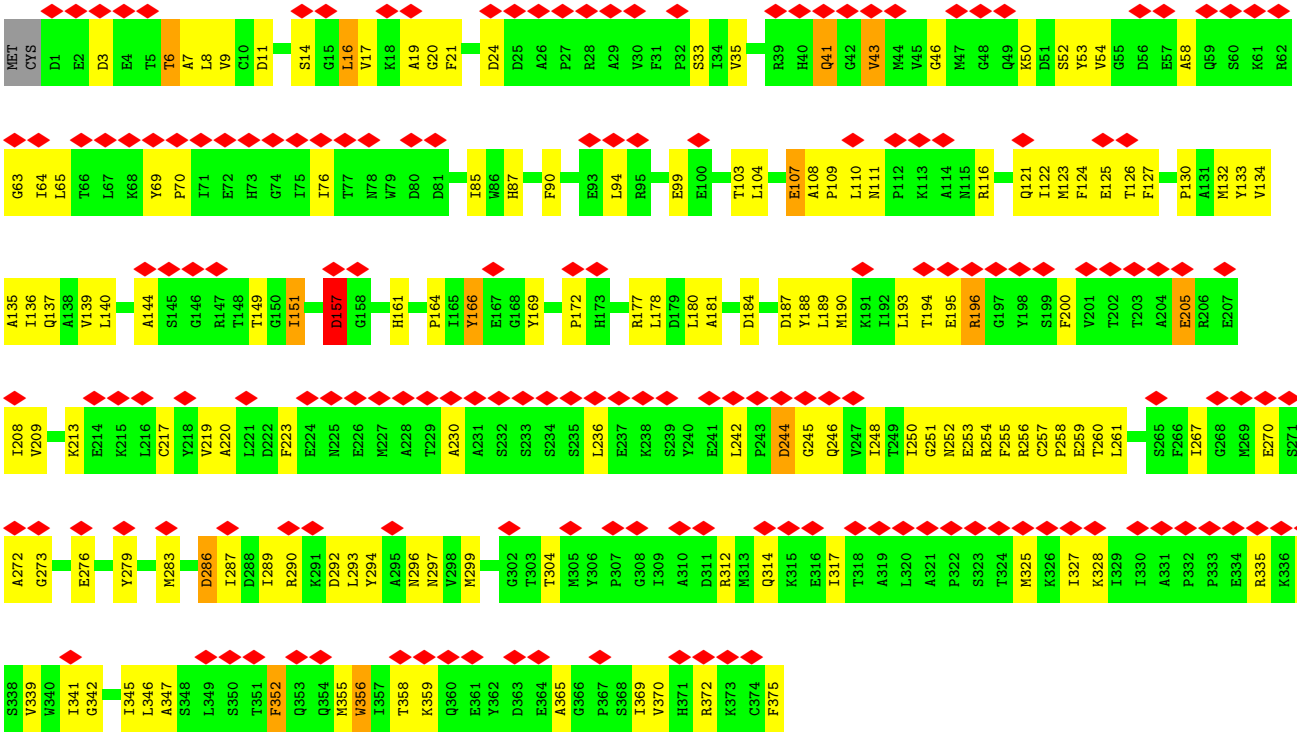
• Molecule 1: Actin, alpha skeletal muscle

Chain B:



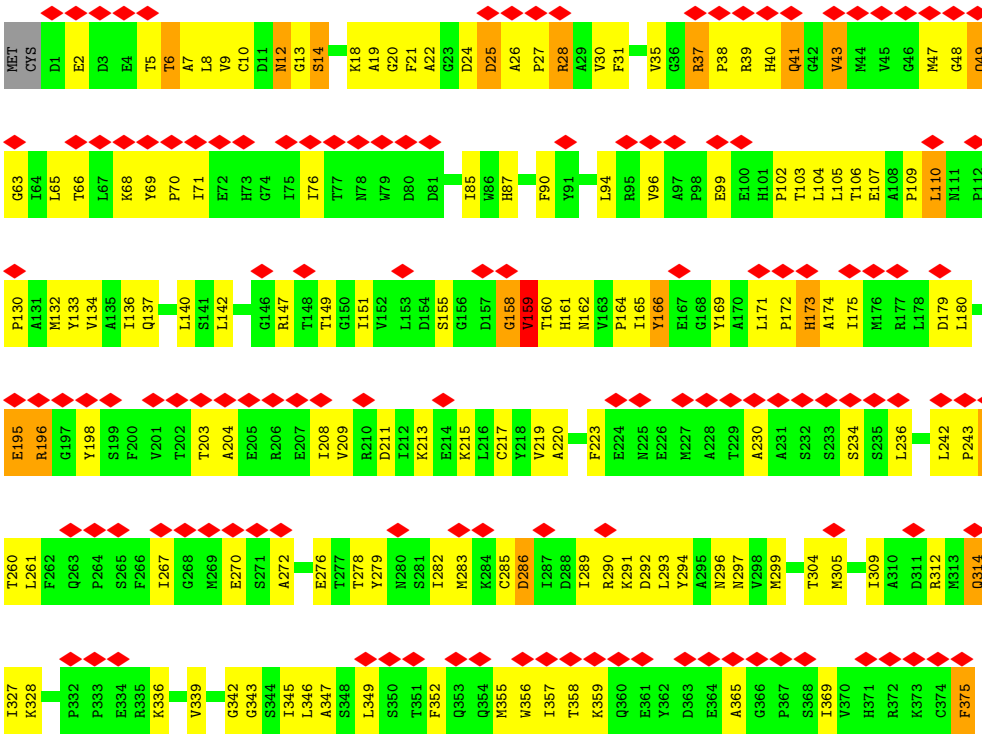
• Molecule 1: Actin, alpha skeletal muscle

Chain C:



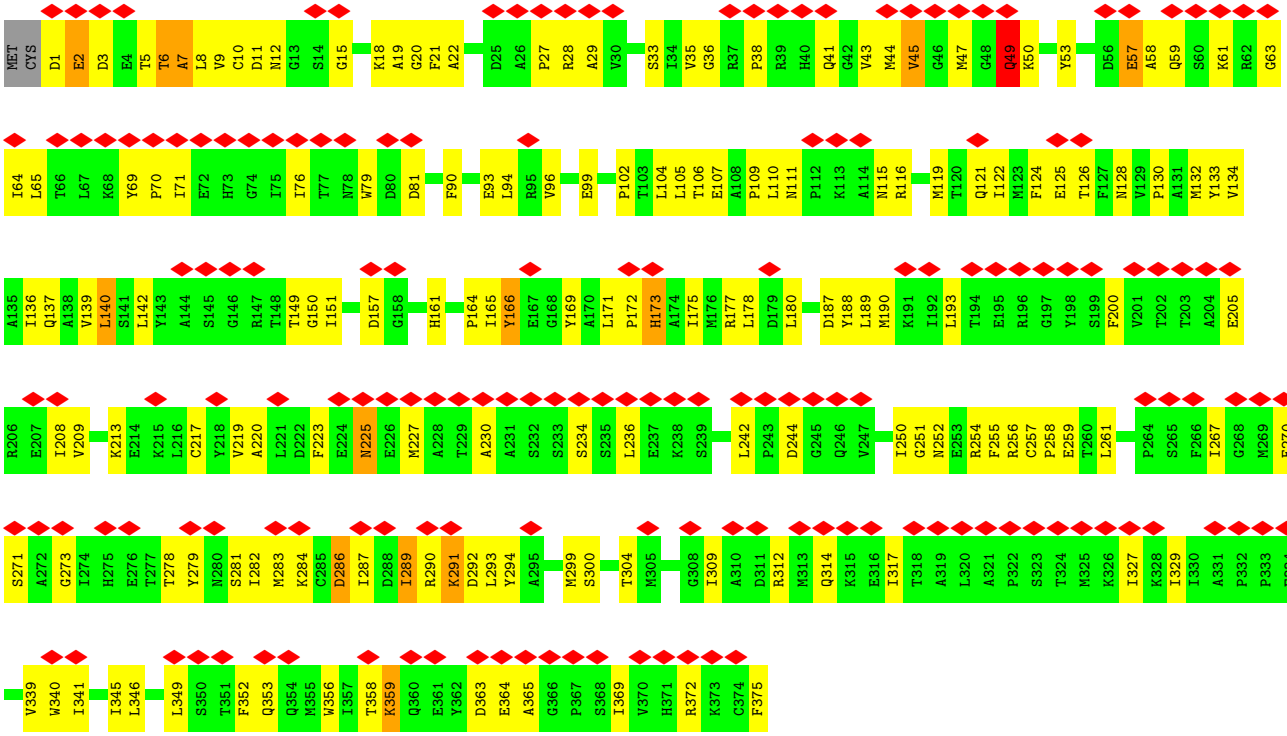
• Molecule 1: Actin, alpha skeletal muscle

Chain D:



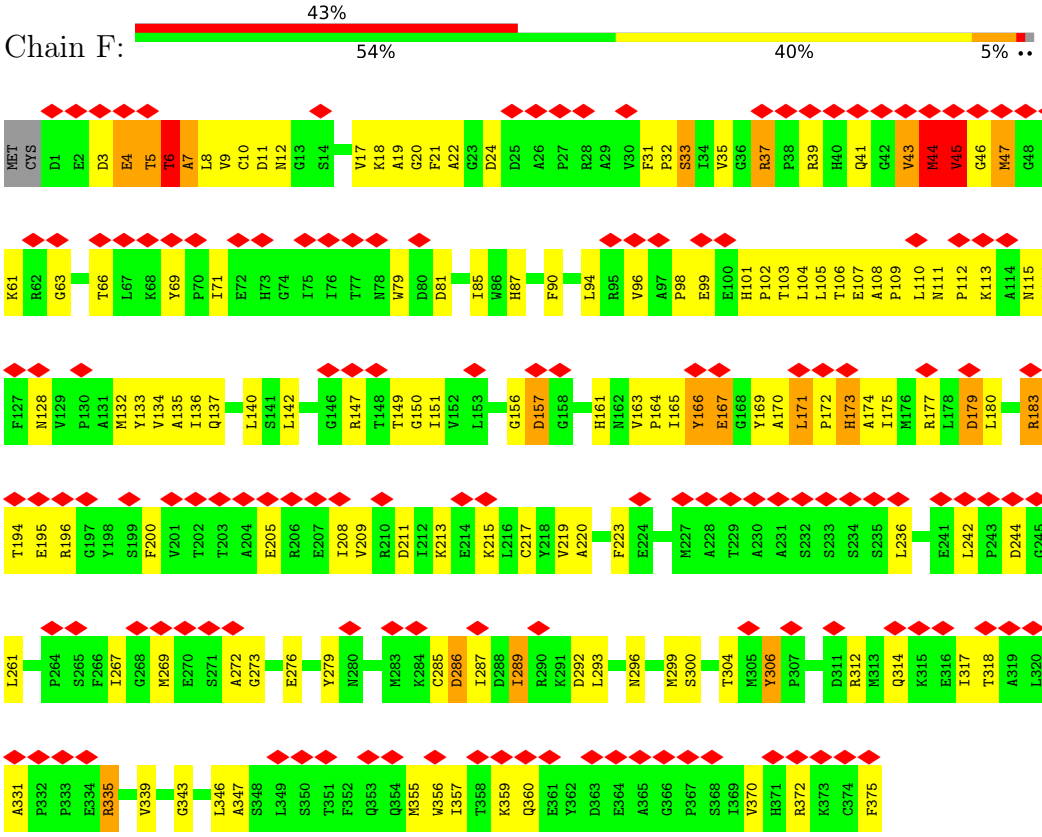
• Molecule 1: Actin, alpha skeletal muscle

Chain E:



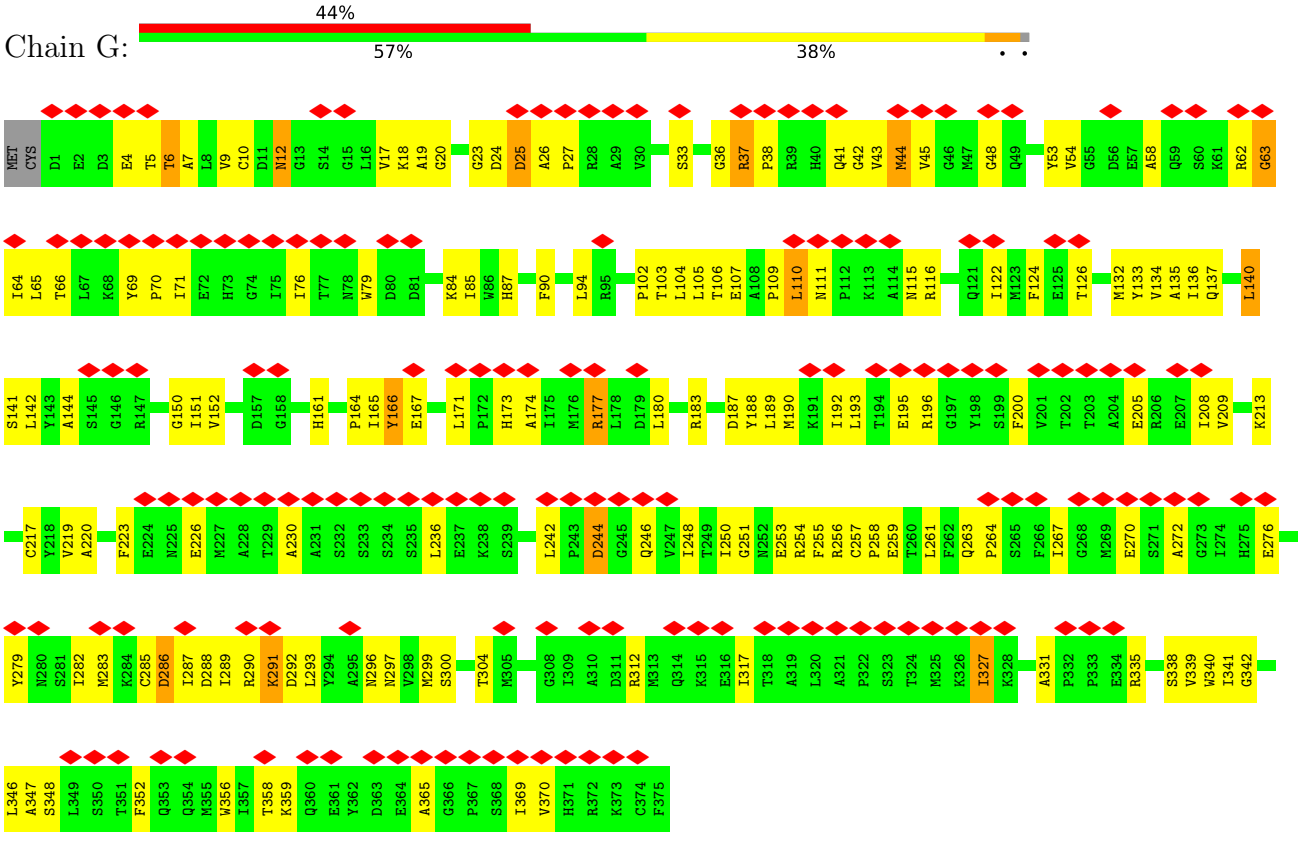
• Molecule 1: Actin, alpha skeletal muscle

Chain F:



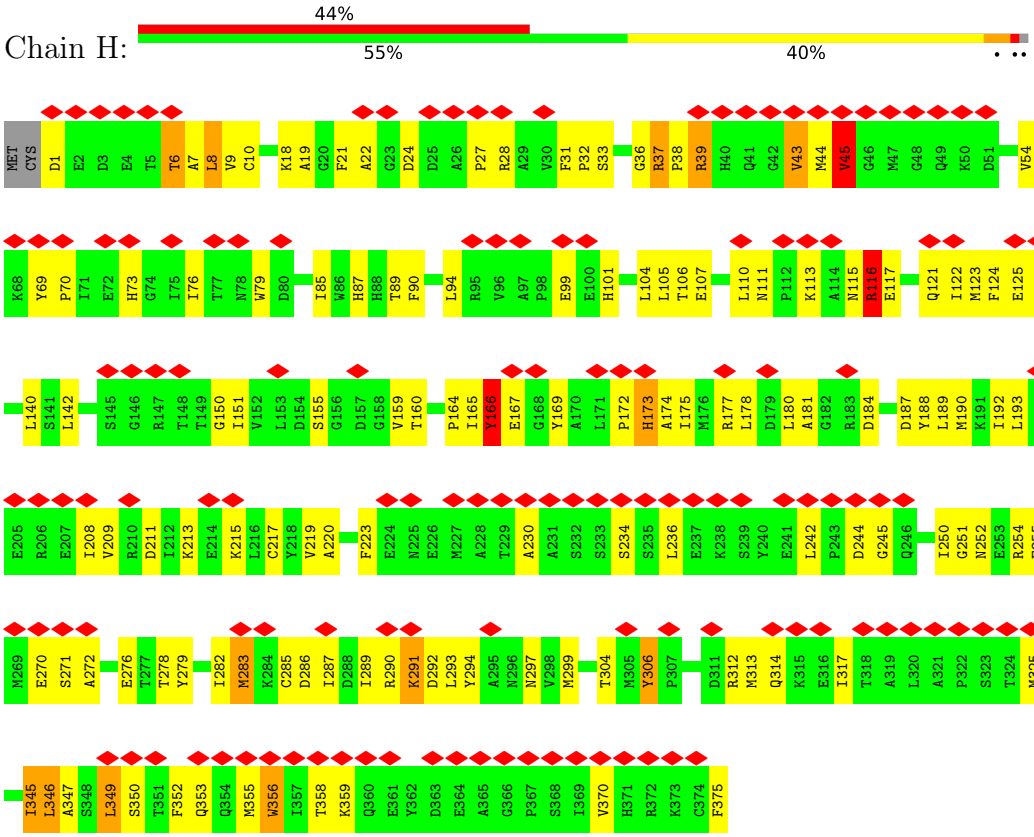
• Molecule 1: Actin, alpha skeletal muscle

Chain G:



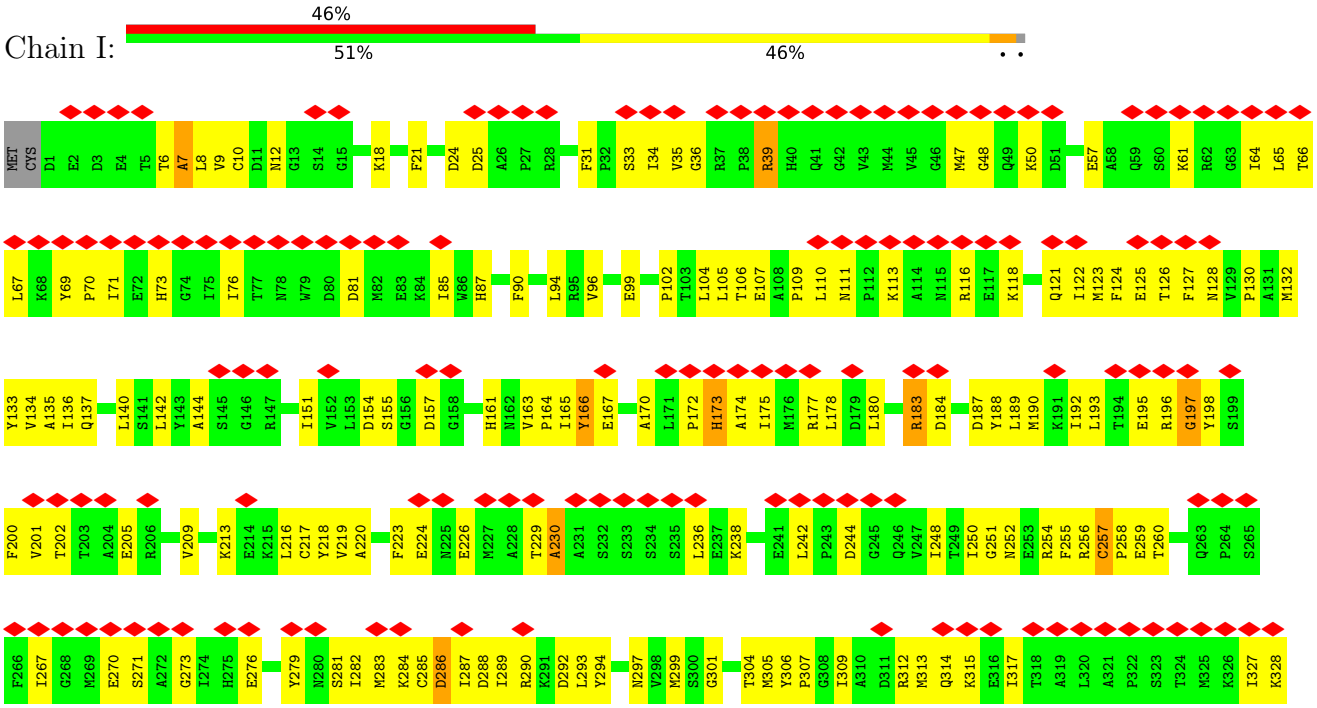
• Molecule 1: Actin, alpha skeletal muscle

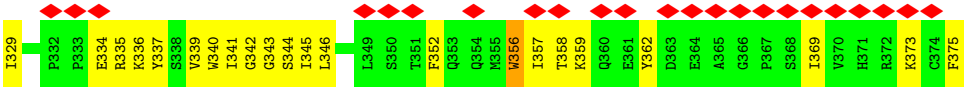
Chain H:



• Molecule 1: Actin, alpha skeletal muscle

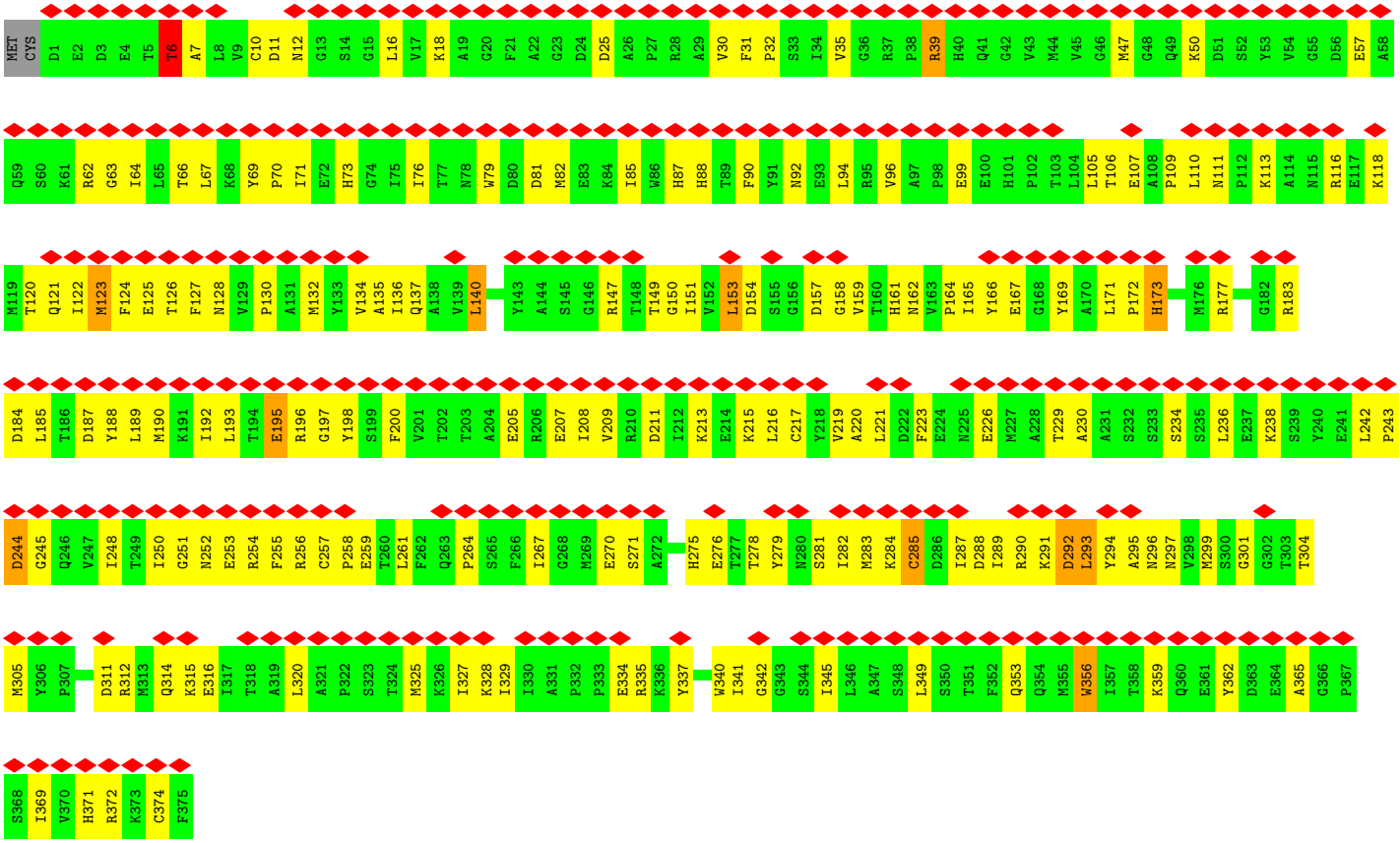
Chain I:





• Molecule 1: Actin, alpha skeletal muscle

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	250.0, 250.0, 250.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5, 2.5, 2.5	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/2996	0.63	0/4058
1	B	0.42	0/2996	0.66	1/4058 (0.0%)
1	C	0.41	0/2996	0.64	0/4058
1	D	0.42	0/2996	0.66	0/4058
1	E	0.40	0/2996	0.65	0/4058
1	F	0.41	0/2996	0.64	0/4058
1	G	0.43	0/2996	0.66	0/4058
1	H	0.44	0/2996	0.68	1/4058 (0.0%)
1	I	0.40	0/2996	0.60	0/4058
1	J	0.38	0/2996	0.58	0/4058
All	All	0.41	0/29960	0.64	2/40580 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	116	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	362	TYR	CB-CG-CD1	-5.20	117.88	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2933	0	2894	113	0
1	C	2933	0	2894	121	0
1	D	2933	0	2894	149	0
1	E	2933	0	2894	126	0
1	F	2933	0	2894	140	0
1	G	2933	0	2894	140	0
1	H	2933	0	2894	150	0
1	I	2933	0	2894	148	0
1	J	2933	0	2894	164	0
All	All	29330	0	28940	1317	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 23.

All (1317) 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:A:63:GLY:HA3	1:C:287:ILE:HG21	1.34	1.06
1:B:7:ALA:HB1	1:B:104:LEU:HB2	1.40	1.00
1:G:58:ALA:HB1	1:G:65:LEU:HD21	1.46	0.97
1:C:58:ALA:HB1	1:C:65:LEU:HD21	1.47	0.95
1:H:151:ILE:HB	1:H:293:LEU:HD22	1.48	0.95
1:A:6:THR:HG22	1:A:22:ALA:HB3	1.45	0.95
1:C:180:LEU:HD21	1:C:261:LEU:HA	1.45	0.94
1:J:151:ILE:HB	1:J:293:LEU:HD13	1.49	0.94
1:I:144:ALA:HB2	1:I:342:GLY:HA2	1.47	0.94
1:I:151:ILE:HB	1:I:293:LEU:HD22	1.50	0.91
1:H:58:ALA:HB1	1:H:65:LEU:HD21	1.48	0.91
1:B:140:LEU:HG	1:B:346:LEU:HD11	1.53	0.90
1:H:289:ILE:HG22	1:H:293:LEU:HG	1.52	0.89
1:H:299:MET:HB3	1:H:304:THR:HG21	1.53	0.87
1:C:64:ILE:HD11	1:E:286:ASP:HB2	1.56	0.87
1:E:6:THR:HG22	1:E:22:ALA:HB3	1.58	0.86
1:H:188:TYR:CE1	1:H:267:ILE:HG22	2.10	0.86
1:B:9:VAL:HG22	1:B:104:LEU:HD23	1.57	0.85
1:D:43:VAL:HG21	1:F:171:LEU:HD11	1.58	0.84
1:A:90:PHE:HA	1:A:94:LEU:HD12	1.59	0.84
1:A:58:ALA:HB1	1:A:65:LEU:HD21	1.60	0.83
1:E:58:ALA:HB1	1:E:65:LEU:HD21	1.61	0.83
1:D:136:ILE:O	1:D:140:LEU:HD13	1.79	0.83
1:G:63:GLY:HA3	1:I:287:ILE:HG21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:ASP:HB3	1:I:289:ILE:HD12	1.59	0.82
1:D:188:TYR:CE1	1:D:267:ILE:HG22	2.13	0.82
1:I:289:ILE:HG22	1:I:293:LEU:HG	1.62	0.82
1:D:5:THR:O	1:D:102:PRO:HG3	1.79	0.82
1:E:90:PHE:HA	1:E:94:LEU:HD12	1.60	0.81
1:E:151:ILE:HB	1:E:293:LEU:HD22	1.61	0.81
1:B:90:PHE:HA	1:B:94:LEU:HD12	1.62	0.81
1:C:286:ASP:HB2	1:C:289:ILE:HD12	1.63	0.81
1:E:180:LEU:HD21	1:E:261:LEU:HA	1.60	0.80
1:C:149:THR:HG21	1:C:292:ASP:HB2	1.61	0.80
1:D:47:MET:HG2	1:D:50:LYS:O	1.81	0.80
1:G:116:ARG:HG2	1:G:370:VAL:HG11	1.63	0.80
1:D:124:PHE:CE1	1:D:132:MET:HG2	2.17	0.80
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.63	0.80
1:F:164:PRO:HB3	1:F:285:CYS:SG	2.22	0.80
1:I:250:ILE:HD12	1:I:254:ARG:HG2	1.64	0.79
1:F:7:ALA:O	1:F:22:ALA:HB2	1.83	0.79
1:I:122:ILE:O	1:I:126:THR:HB	1.83	0.79
1:F:111:ASN:HB3	1:F:116:ARG:NH1	1.99	0.78
1:F:180:LEU:HD21	1:F:261:LEU:HA	1.63	0.78
1:F:250:ILE:HD12	1:F:254:ARG:HG2	1.65	0.78
1:C:299:MET:HB3	1:C:304:THR:HG21	1.66	0.78
1:C:188:TYR:CE1	1:C:267:ILE:HG22	2.19	0.77
1:J:99:GLU:HA	1:J:128:ASN:O	1.84	0.77
1:J:287:ILE:HD13	1:J:290:ARG:HH12	1.48	0.77
1:B:137:GLN:HG3	1:B:339:VAL:HG13	1.67	0.77
1:F:9:VAL:O	1:F:19:ALA:HA	1.84	0.77
1:J:236:LEU:O	1:J:251:GLY:HA2	1.85	0.77
1:B:58:ALA:HB1	1:B:65:LEU:HD21	1.66	0.77
1:I:230:ALA:HA	1:I:236:LEU:HD22	1.67	0.77
1:B:261:LEU:HD11	1:B:303:THR:HG22	1.65	0.76
1:C:151:ILE:HG12	1:C:293:LEU:HD22	1.67	0.76
1:H:43:VAL:HG12	1:H:44:MET:H	1.48	0.76
1:H:187:ASP:O	1:H:190:MET:HG2	1.85	0.76
1:H:236:LEU:O	1:H:251:GLY:HA2	1.85	0.76
1:H:54:VAL:HG21	1:H:85:ILE:HA	1.67	0.76
1:I:236:LEU:O	1:I:251:GLY:HA2	1.85	0.76
1:D:174:ALA:HB1	1:D:285:CYS:SG	2.25	0.76
1:F:44:MET:O	1:F:45:VAL:HB	1.86	0.76
1:H:136:ILE:O	1:H:140:LEU:HD13	1.86	0.75
1:H:250:ILE:HD12	1:H:254:ARG:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:O	1:C:140:LEU:HD13	1.86	0.75
1:A:286:ASP:HB3	1:A:289:ILE:HD12	1.69	0.75
1:A:136:ILE:O	1:A:140:LEU:HD13	1.86	0.75
1:F:103:THR:O	1:F:132:MET:HB2	1.85	0.75
1:J:230:ALA:HA	1:J:236:LEU:HD22	1.67	0.75
1:A:187:ASP:O	1:A:190:MET:HG2	1.86	0.75
1:D:164:PRO:HB3	1:D:285:CYS:SG	2.27	0.75
1:G:187:ASP:O	1:G:190:MET:HG2	1.86	0.75
1:H:180:LEU:HD21	1:H:261:LEU:HA	1.68	0.75
1:I:107:GLU:HB2	1:I:134:VAL:HG22	1.67	0.75
1:C:137:GLN:HG3	1:C:339:VAL:HG13	1.68	0.75
1:C:219:VAL:HG22	1:C:258:PRO:HB3	1.69	0.75
1:C:250:ILE:HD12	1:C:254:ARG:HG2	1.69	0.74
1:F:136:ILE:O	1:F:140:LEU:HD13	1.86	0.74
1:G:180:LEU:HD21	1:G:261:LEU:HA	1.69	0.74
1:H:63:GLY:HA3	1:J:288:ASP:H	1.52	0.74
1:H:150:GLY:O	1:H:165:ILE:HG21	1.87	0.74
1:C:194:THR:HG21	1:D:171:LEU:HD13	1.68	0.74
1:E:150:GLY:O	1:E:165:ILE:HB	1.88	0.74
1:E:133:TYR:CD1	1:E:356:TRP:HA	2.22	0.74
1:H:286:ASP:HB2	1:H:289:ILE:HD12	1.69	0.74
1:E:187:ASP:O	1:E:190:MET:HG2	1.88	0.74
1:I:135:ALA:HB1	1:I:140:LEU:HD11	1.69	0.74
1:H:136:ILE:HD13	1:H:375:PHE:CD1	2.22	0.74
1:E:164:PRO:HD2	1:E:175:ILE:HG22	1.70	0.73
1:B:124:PHE:CE1	1:B:132:MET:HG2	2.23	0.73
1:J:287:ILE:HA	1:J:290:ARG:NH1	2.02	0.73
1:B:289:ILE:HG22	1:B:293:LEU:HD11	1.70	0.73
1:B:346:LEU:HD13	1:B:352:PHE:CE1	2.23	0.73
1:G:26:ALA:HB1	1:G:27:PRO:HD2	1.71	0.73
1:B:99:GLU:HG3	1:B:127:PHE:O	1.89	0.73
1:B:122:ILE:O	1:B:126:THR:HB	1.89	0.73
1:E:27:PRO:HD3	1:E:340:TRP:CZ2	2.24	0.73
1:H:208:ILE:HG21	1:H:242:LEU:HD11	1.70	0.73
1:D:187:ASP:O	1:D:190:MET:HG2	1.88	0.72
1:E:299:MET:HB3	1:E:304:THR:HG21	1.70	0.72
1:H:164:PRO:HB3	1:H:285:CYS:SG	2.28	0.72
1:E:289:ILE:HG22	1:E:293:LEU:HG	1.71	0.72
1:C:136:ILE:HD13	1:C:375:PHE:CE1	2.25	0.72
1:D:137:GLN:HG3	1:D:339:VAL:HG13	1.71	0.72
1:I:187:ASP:O	1:I:190:MET:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:TYR:HD2	1:I:257:CYS:HG	1.37	0.72
1:A:236:LEU:O	1:A:251:GLY:HA2	1.90	0.72
1:H:164:PRO:HD2	1:H:175:ILE:HG22	1.72	0.71
1:F:90:PHE:HA	1:F:94:LEU:HD12	1.71	0.71
1:F:120:THR:HA	1:F:132:MET:CE	2.19	0.71
1:F:150:GLY:O	1:F:165:ILE:HB	1.88	0.71
1:H:116:ARG:HH11	1:H:116:ARG:CG	2.04	0.71
1:F:151:ILE:HB	1:F:293:LEU:HD22	1.72	0.71
1:I:289:ILE:HG22	1:I:293:LEU:CG	2.20	0.71
1:D:236:LEU:O	1:D:251:GLY:HA2	1.91	0.71
1:D:365:ALA:HB3	1:D:369:ILE:HD13	1.72	0.71
1:G:111:ASN:HB3	1:G:116:ARG:NH1	2.06	0.71
1:D:21:PHE:HB2	1:D:24:ASP:OD2	1.91	0.71
1:G:110:LEU:HD21	1:G:177:ARG:HD3	1.71	0.71
1:H:104:LEU:HD22	1:H:347:ALA:HB2	1.72	0.71
1:C:116:ARG:HB3	1:C:370:VAL:HG21	1.73	0.70
1:F:285:CYS:O	1:F:286:ASP:HB2	1.90	0.70
1:H:289:ILE:HG22	1:H:293:LEU:CG	2.19	0.70
1:F:10:CYS:HA	1:F:18:LYS:O	1.91	0.70
1:H:124:PHE:CE1	1:H:132:MET:HG2	2.26	0.70
1:B:142:LEU:HD22	1:B:165:ILE:HG12	1.73	0.70
1:G:27:PRO:HD3	1:G:340:TRP:CZ3	2.27	0.70
1:C:124:PHE:CE1	1:C:132:MET:HG2	2.27	0.70
1:A:122:ILE:O	1:A:126:THR:HB	1.90	0.70
1:F:3:ASP:O	1:F:4:GLU:HB2	1.90	0.70
1:F:137:GLN:HG3	1:F:339:VAL:HG11	1.74	0.70
1:F:200:PHE:HA	1:F:205:GLU:OE2	1.92	0.70
1:G:133:TYR:CD1	1:G:356:TRP:HA	2.26	0.70
1:A:140:LEU:HG	1:A:346:LEU:CD1	2.22	0.70
1:F:213:LYS:O	1:F:217:CYS:HB2	1.92	0.70
1:G:124:PHE:CE1	1:G:132:MET:HG2	2.27	0.70
1:G:286:ASP:HB3	1:G:289:ILE:HD12	1.74	0.70
1:D:314:GLN:OE1	1:D:328:LYS:HA	1.92	0.70
1:G:109:PRO:O	1:G:110:LEU:HD13	1.92	0.69
1:B:140:LEU:CG	1:B:346:LEU:HD11	2.20	0.69
1:J:250:ILE:HD12	1:J:254:ARG:HG2	1.73	0.69
1:D:213:LYS:O	1:D:217:CYS:HB2	1.93	0.69
1:C:99:GLU:HG3	1:C:127:PHE:O	1.93	0.69
1:G:338:SER:HA	1:G:341:ILE:HG22	1.75	0.69
1:A:166:TYR:CD1	1:A:289:ILE:HG23	2.27	0.69
1:B:116:ARG:HG2	1:B:370:VAL:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:PHE:CE1	1:E:132:MET:HG2	2.28	0.69
1:E:208:ILE:HG21	1:E:242:LEU:HD11	1.75	0.69
1:G:136:ILE:O	1:G:140:LEU:HD13	1.91	0.69
1:J:107:GLU:HB2	1:J:134:VAL:HG22	1.73	0.69
1:J:289:ILE:HG22	1:J:293:LEU:HD23	1.73	0.69
1:C:213:LYS:O	1:C:217:CYS:HB2	1.93	0.69
1:E:279:TYR:OH	1:E:317:ILE:HA	1.92	0.69
1:F:236:LEU:O	1:F:251:GLY:HA2	1.93	0.69
1:G:289:ILE:HG22	1:G:293:LEU:HG	1.75	0.69
1:J:122:ILE:O	1:J:126:THR:HB	1.92	0.69
1:C:208:ILE:HG21	1:C:242:LEU:HD11	1.75	0.69
1:C:289:ILE:HG22	1:C:293:LEU:HG	1.74	0.69
1:A:99:GLU:HG2	1:A:127:PHE:O	1.93	0.68
1:H:10:CYS:HA	1:H:18:LYS:O	1.93	0.68
1:E:137:GLN:HG3	1:E:339:VAL:HG13	1.74	0.68
1:F:187:ASP:O	1:F:190:MET:HG2	1.92	0.68
1:A:242:LEU:HD23	1:A:244:ASP:H	1.58	0.68
1:A:287:ILE:HD13	1:A:290:ARG:HH12	1.58	0.68
1:A:111:ASN:HB3	1:A:116:ARG:NH1	2.09	0.68
1:A:136:ILE:HD13	1:A:375:PHE:HE1	1.57	0.68
1:D:40:HIS:O	1:D:41:GLN:HG2	1.92	0.68
1:G:188:TYR:CE1	1:G:267:ILE:HG22	2.29	0.68
1:G:236:LEU:O	1:G:251:GLY:HA2	1.94	0.68
1:B:187:ASP:O	1:B:190:MET:HG2	1.93	0.68
1:B:208:ILE:HG21	1:B:242:LEU:HD11	1.74	0.68
1:D:35:VAL:O	1:D:68:LYS:HB3	1.94	0.68
1:B:166:TYR:CE1	1:B:289:ILE:HG12	2.30	0.67
1:H:213:LYS:O	1:H:217:CYS:HB2	1.94	0.67
1:I:39:ARG:HG3	1:I:64:ILE:O	1.93	0.67
1:I:197:GLY:HA2	1:J:113:LYS:CB	2.23	0.67
1:J:151:ILE:CB	1:J:293:LEU:HD13	2.23	0.67
1:E:8:LEU:HG	1:E:20:GLY:O	1.94	0.67
1:E:353:GLN:HA	1:E:356:TRP:CZ2	2.28	0.67
1:A:149:THR:HG23	1:A:166:TYR:HA	1.77	0.67
1:C:124:PHE:CZ	1:C:132:MET:HG2	2.29	0.67
1:H:107:GLU:HB2	1:H:134:VAL:HG22	1.75	0.67
1:E:236:LEU:O	1:E:251:GLY:HA2	1.93	0.67
1:I:219:VAL:HG22	1:I:258:PRO:HB3	1.75	0.67
1:B:250:ILE:HD12	1:B:254:ARG:HG2	1.77	0.67
1:H:27:PRO:HD3	1:H:340:TRP:CH2	2.30	0.67
1:C:90:PHE:HA	1:C:94:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:ILE:HD12	1:G:327:ILE:N	2.09	0.67
1:A:287:ILE:HA	1:A:290:ARG:NH1	2.08	0.67
1:J:337:TYR:O	1:J:341:ILE:HG12	1.95	0.67
1:I:142:LEU:HD22	1:I:165:ILE:HG21	1.77	0.67
1:I:170:ALA:O	1:I:375:PHE:HB3	1.96	0.67
1:B:71:ILE:HG12	1:B:76:ILE:HG12	1.77	0.66
1:G:213:LYS:O	1:G:217:CYS:HB2	1.94	0.66
1:J:50:LYS:HG3	1:J:57:GLU:OE1	1.94	0.66
1:J:187:ASP:O	1:J:190:MET:HG2	1.93	0.66
1:C:187:ASP:O	1:C:190:MET:HG2	1.95	0.66
1:I:220:ALA:O	1:I:312:ARG:HD2	1.95	0.66
1:D:219:VAL:HG22	1:D:258:PRO:HB3	1.77	0.66
1:H:116:ARG:HD3	1:H:370:VAL:HG11	1.77	0.66
1:C:41:GLN:HG2	1:C:43:VAL:H	1.59	0.66
1:E:7:ALA:O	1:E:22:ALA:HB2	1.96	0.66
1:G:188:TYR:CD1	1:G:267:ILE:HG22	2.30	0.66
1:H:270:GLU:HG3	1:H:271:SER:N	2.11	0.65
1:F:37:ARG:O	1:F:66:THR:HG23	1.96	0.65
1:F:188:TYR:CD1	1:F:267:ILE:HG22	2.31	0.65
1:C:188:TYR:CD1	1:C:267:ILE:HG22	2.31	0.65
1:D:282:ILE:CG2	1:D:290:ARG:HG2	2.26	0.65
1:F:120:THR:HA	1:F:132:MET:HE2	1.78	0.65
1:A:250:ILE:HD12	1:A:254:ARG:HG2	1.77	0.65
1:C:236:LEU:O	1:C:251:GLY:HA2	1.96	0.65
1:F:140:LEU:HG	1:F:346:LEU:HD12	1.79	0.65
1:H:63:GLY:CA	1:J:288:ASP:H	2.10	0.65
1:H:314:GLN:HE21	1:H:329:ILE:HG12	1.62	0.65
1:A:10:CYS:HA	1:A:18:LYS:O	1.97	0.65
1:E:111:ASN:HB3	1:E:116:ARG:NH1	2.11	0.65
1:B:188:TYR:CE1	1:B:267:ILE:HG22	2.31	0.65
1:B:236:LEU:O	1:B:251:GLY:HA2	1.95	0.65
1:I:70:PRO:O	1:I:76:ILE:HA	1.96	0.65
1:A:149:THR:HG21	1:A:292:ASP:OD2	1.97	0.65
1:J:25:ASP:O	1:J:341:ILE:HD12	1.97	0.64
1:C:289:ILE:HG22	1:C:293:LEU:CG	2.27	0.64
1:H:1:ASP:HB3	1:H:101:HIS:CE1	2.33	0.64
1:A:213:LYS:O	1:A:217:CYS:HB2	1.96	0.64
1:C:149:THR:HG22	1:C:296:ASN:HD22	1.62	0.64
1:D:124:PHE:CE2	1:D:359:LYS:HB2	2.33	0.64
1:D:90:PHE:HA	1:D:94:LEU:HD12	1.77	0.64
1:D:142:LEU:HD22	1:D:165:ILE:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:PRO:HG2	1:F:115:ASN:OD1	1.97	0.64
1:C:50:LYS:HG3	1:C:52:SER:O	1.98	0.64
1:E:188:TYR:CE1	1:E:267:ILE:HG22	2.33	0.64
1:G:107:GLU:HB2	1:G:134:VAL:HG22	1.78	0.64
1:H:314:GLN:NE2	1:H:329:ILE:HG12	2.12	0.64
1:I:136:ILE:O	1:I:140:LEU:HD13	1.97	0.64
1:B:7:ALA:CB	1:B:104:LEU:HB2	2.24	0.64
1:B:151:ILE:HD12	1:B:164:PRO:HA	1.79	0.64
1:G:166:TYR:CZ	1:G:289:ILE:HG12	2.32	0.64
1:D:289:ILE:O	1:D:293:LEU:HG	1.96	0.64
1:E:63:GLY:HA3	1:G:287:ILE:HG21	1.78	0.64
1:D:99:GLU:HA	1:D:128:ASN:O	1.97	0.63
1:E:12:ASN:HD21	1:E:71:ILE:HD11	1.62	0.63
1:C:149:THR:CG2	1:C:292:ASP:HB2	2.28	0.63
1:E:142:LEU:HD22	1:E:165:ILE:CG2	2.28	0.63
1:F:194:THR:HG21	1:G:171:LEU:HD11	1.79	0.63
1:G:250:ILE:HA	1:G:253:GLU:OE2	1.98	0.63
1:J:220:ALA:O	1:J:312:ARG:HD2	1.99	0.63
1:J:276:GLU:HA	1:J:279:TYR:CD1	2.34	0.63
1:C:289:ILE:O	1:C:293:LEU:HG	1.97	0.63
1:F:136:ILE:HG21	1:F:375:PHE:CZ	2.34	0.63
1:H:122:ILE:O	1:H:126:THR:HB	1.98	0.63
1:D:43:VAL:HG21	1:F:171:LEU:CD1	2.29	0.62
1:H:164:PRO:HG3	1:H:174:ALA:HB3	1.81	0.62
1:B:107:GLU:HB2	1:B:134:VAL:HG22	1.81	0.62
1:D:142:LEU:HD22	1:D:165:ILE:CG2	2.29	0.62
1:B:29:ALA:HB2	1:B:93:GLU:HB2	1.82	0.62
1:G:299:MET:HB3	1:G:304:THR:HG21	1.80	0.62
1:E:200:PHE:HA	1:E:205:GLU:OE2	2.00	0.62
1:G:151:ILE:HB	1:G:293:LEU:HD22	1.81	0.62
1:I:285:CYS:O	1:I:286:ASP:HB2	1.99	0.62
1:I:286:ASP:HB3	1:I:289:ILE:CD1	2.28	0.62
1:G:116:ARG:HB3	1:G:370:VAL:HG21	1.80	0.62
1:G:250:ILE:HD12	1:G:254:ARG:HG2	1.80	0.62
1:I:50:LYS:HG3	1:I:57:GLU:OE1	2.00	0.62
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.81	0.62
1:G:248:ILE:HG22	1:G:250:ILE:HG23	1.82	0.62
1:J:151:ILE:HG22	1:J:297:ASN:HD22	1.65	0.62
1:E:213:LYS:O	1:E:217:CYS:HB2	2.00	0.62
1:H:36:GLY:HA3	1:H:65:LEU:HG	1.82	0.62
1:E:250:ILE:HD12	1:E:254:ARG:HG2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:TYR:CD2	1:I:289:ILE:HG12	2.35	0.61
1:J:294:TYR:HB3	1:J:327:ILE:HD13	1.81	0.61
1:B:111:ASN:HB3	1:B:116:ARG:NH1	2.15	0.61
1:C:111:ASN:HB3	1:C:116:ARG:NH1	2.15	0.61
1:C:116:ARG:CB	1:C:370:VAL:HG21	2.30	0.61
1:F:286:ASP:HB3	1:F:289:ILE:HG13	1.82	0.61
1:B:136:ILE:HD11	1:B:374:CYS:HB2	1.81	0.61
1:B:213:LYS:O	1:B:217:CYS:HB2	2.00	0.61
1:I:166:TYR:CE2	1:I:289:ILE:HG12	2.35	0.61
1:F:189:LEU:O	1:F:193:LEU:HD13	2.01	0.61
1:F:318:THR:HG22	1:F:327:ILE:HD12	1.83	0.61
1:A:7:ALA:O	1:A:22:ALA:HB2	2.00	0.61
1:H:45:VAL:HG21	1:J:169:TYR:H	1.66	0.61
1:J:353:GLN:HG3	1:J:356:TRP:CZ2	2.36	0.61
1:D:53:TYR:HB2	1:D:65:LEU:HD21	1.82	0.61
1:F:223:PHE:CD1	1:F:259:GLU:HG2	2.35	0.61
1:J:213:LYS:O	1:J:217:CYS:HB2	2.00	0.61
1:G:20:GLY:HA2	1:G:94:LEU:HD21	1.82	0.61
1:H:8:LEU:HD21	1:H:90:PHE:CE1	2.36	0.61
1:H:9:VAL:HG13	1:H:104:LEU:HD23	1.83	0.61
1:H:133:TYR:CD1	1:H:356:TRP:HA	2.36	0.61
1:F:6:THR:HG22	1:F:22:ALA:HB3	1.83	0.61
1:J:283:MET:HA	1:J:290:ARG:NH2	2.15	0.61
1:B:8:LEU:HD21	1:B:90:PHE:HE1	1.66	0.60
1:D:188:TYR:CD1	1:D:267:ILE:HG22	2.36	0.60
1:A:305:MET:SD	1:A:336:LYS:HB2	2.40	0.60
1:D:166:TYR:CE2	1:D:289:ILE:HG12	2.37	0.60
1:H:111:ASN:HB3	1:H:116:ARG:NH1	2.16	0.60
1:J:90:PHE:HA	1:J:94:LEU:HD12	1.82	0.60
1:B:156:GLY:O	1:B:157:ASP:HB2	2.00	0.60
1:D:345:ILE:O	1:D:349:LEU:HG	2.02	0.60
1:H:195:GLU:HG3	1:H:196:ARG:N	2.16	0.60
1:B:21:PHE:HB2	1:B:24:ASP:OD1	2.02	0.60
1:C:9:VAL:O	1:C:19:ALA:HA	2.02	0.60
1:G:208:ILE:HG21	1:G:242:LEU:HD11	1.83	0.60
1:I:34:ILE:HD12	1:I:67:LEU:HD22	1.83	0.60
1:E:124:PHE:CZ	1:E:132:MET:HG2	2.37	0.60
1:B:189:LEU:O	1:B:193:LEU:HD13	2.02	0.60
1:H:63:GLY:HA2	1:J:287:ILE:H	1.67	0.60
1:H:223:PHE:HB2	1:H:259:GLU:CD	2.22	0.60
1:G:4:GLU:HG3	1:G:5:THR:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:ALA:HB2	1:I:342:GLY:CA	2.27	0.60
1:I:183:ARG:HG3	1:I:184:ASP:N	2.15	0.60
1:I:279:TYR:OH	1:I:317:ILE:HA	2.01	0.60
1:D:250:ILE:HD12	1:D:254:ARG:HG2	1.82	0.60
1:F:11:ASP:OD1	1:F:106:THR:HG21	2.01	0.60
1:F:321:ALA:HB1	1:F:322:PRO:HD2	1.84	0.60
1:J:136:ILE:O	1:J:140:LEU:HD13	2.01	0.60
1:G:142:LEU:HD22	1:G:165:ILE:HG12	1.83	0.60
1:E:5:THR:O	1:E:102:PRO:HG2	2.02	0.60
1:F:331:ALA:HB1	1:F:335:ARG:HH11	1.65	0.60
1:C:116:ARG:HG2	1:C:370:VAL:HG11	1.83	0.59
1:I:201:VAL:HG21	1:J:110:LEU:HD13	1.83	0.59
1:J:164:PRO:HB3	1:J:285:CYS:SG	2.42	0.59
1:A:71:ILE:HD13	1:A:76:ILE:HG12	1.83	0.59
1:H:219:VAL:HG12	1:H:312:ARG:HD2	1.84	0.59
1:F:289:ILE:HG22	1:F:293:LEU:HG	1.84	0.59
1:A:220:ALA:HB1	1:A:226:GLU:OE2	2.02	0.59
1:C:7:ALA:HB1	1:C:104:LEU:HB2	1.83	0.59
1:H:286:ASP:HB2	1:H:289:ILE:CD1	2.32	0.59
1:B:140:LEU:CD1	1:B:346:LEU:HD11	2.32	0.59
1:D:10:CYS:HA	1:D:18:LYS:O	2.02	0.59
1:D:223:PHE:HB2	1:D:259:GLU:CD	2.23	0.59
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.83	0.59
1:F:5:THR:HB	1:F:102:PRO:HG2	1.85	0.59
1:F:124:PHE:CE1	1:F:132:MET:HG2	2.38	0.59
1:F:136:ILE:HD13	1:F:375:PHE:CE1	2.38	0.59
1:G:289:ILE:HG22	1:G:293:LEU:CG	2.32	0.59
1:H:39:ARG:HB2	1:H:66:THR:HG22	1.85	0.59
1:A:133:TYR:CD1	1:A:356:TRP:HA	2.38	0.59
1:E:9:VAL:O	1:E:19:ALA:HA	2.02	0.59
1:H:61:LYS:HB3	1:J:288:ASP:HB2	1.83	0.59
1:H:195:GLU:HG3	1:H:196:ARG:H	1.68	0.59
1:B:7:ALA:O	1:B:22:ALA:HB2	2.01	0.59
1:C:144:ALA:HB2	1:C:342:GLY:HA2	1.85	0.59
1:D:13:GLY:O	1:D:14:SER:HB2	2.03	0.59
1:D:18:LYS:HG2	1:D:30:VAL:HG12	1.84	0.59
1:H:136:ILE:HD12	1:H:169:TYR:CD2	2.38	0.59
1:H:276:GLU:HA	1:H:279:TYR:CD1	2.38	0.59
1:H:189:LEU:O	1:H:193:LEU:HD13	2.03	0.58
1:C:63:GLY:HA3	1:E:287:ILE:HG21	1.85	0.58
1:G:110:LEU:HD21	1:G:177:ARG:CD	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:ILE:HD12	1:G:327:ILE:H	1.68	0.58
1:F:286:ASP:HB3	1:F:289:ILE:CG1	2.33	0.58
1:G:116:ARG:CG	1:G:370:VAL:HG11	2.34	0.58
1:H:62:ARG:O	1:J:288:ASP:HB3	2.03	0.58
1:H:63:GLY:HA2	1:J:287:ILE:N	2.18	0.58
1:I:136:ILE:HG21	1:I:375:PHE:CZ	2.39	0.58
1:D:26:ALA:HB1	1:D:27:PRO:HD2	1.85	0.58
1:E:70:PRO:O	1:E:76:ILE:HG12	2.04	0.58
1:F:223:PHE:HB2	1:F:259:GLU:CD	2.24	0.58
1:F:279:TYR:OH	1:F:317:ILE:HA	2.03	0.58
1:H:279:TYR:OH	1:H:317:ILE:HA	2.03	0.58
1:A:220:ALA:O	1:A:312:ARG:HD2	2.04	0.58
1:B:261:LEU:HD21	1:B:303:THR:HG21	1.84	0.58
1:D:22:ALA:CB	1:D:347:ALA:HB1	2.34	0.58
1:D:58:ALA:HB1	1:D:65:LEU:HD11	1.84	0.58
1:I:99:GLU:HG3	1:I:127:PHE:O	2.03	0.58
1:J:71:ILE:HG12	1:J:76:ILE:HG12	1.86	0.58
1:J:94:LEU:HB3	1:J:96:VAL:HG22	1.85	0.58
1:F:164:PRO:HG3	1:F:174:ALA:HB3	1.86	0.58
1:D:180:LEU:HD21	1:D:261:LEU:HA	1.85	0.58
1:H:188:TYR:CD1	1:H:267:ILE:HG22	2.39	0.58
1:A:173:HIS:O	1:A:284:LYS:HD3	2.03	0.58
1:A:279:TYR:CE1	1:A:320:LEU:HB2	2.38	0.58
1:D:171:LEU:HA	1:D:375:PHE:HB2	1.85	0.58
1:G:62:ARG:HG2	1:G:63:GLY:H	1.69	0.58
1:G:122:ILE:O	1:G:126:THR:HB	2.03	0.58
1:I:94:LEU:HB3	1:I:96:VAL:HG22	1.85	0.58
1:H:99:GLU:O	1:H:130:PRO:HD3	2.03	0.58
1:H:257:CYS:HB3	1:H:258:PRO:HD3	1.86	0.58
1:B:140:LEU:HG	1:B:346:LEU:CD1	2.31	0.58
1:F:105:LEU:HD13	1:F:119:MET:SD	2.44	0.58
1:J:219:VAL:HG22	1:J:258:PRO:HB3	1.85	0.58
1:B:261:LEU:HD11	1:B:303:THR:CG2	2.34	0.57
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.86	0.57
1:E:189:LEU:O	1:E:193:LEU:HD13	2.04	0.57
1:B:42:GLY:O	1:B:43:VAL:HB	2.03	0.57
1:E:64:ILE:HD11	1:G:286:ASP:OD1	2.04	0.57
1:A:142:LEU:HD22	1:A:165:ILE:HG12	1.86	0.57
1:C:178:LEU:HG	1:C:180:LEU:H	1.69	0.57
1:I:201:VAL:HG11	1:J:177:ARG:HB3	1.86	0.57
1:A:289:ILE:HG22	1:A:293:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD21	1:B:90:PHE:CE1	2.39	0.57
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.87	0.57
1:H:230:ALA:HA	1:H:236:LEU:HD22	1.87	0.57
1:A:136:ILE:HD13	1:A:375:PHE:CE1	2.38	0.57
1:D:189:LEU:O	1:D:193:LEU:HD13	2.04	0.57
1:I:242:LEU:HD23	1:I:244:ASP:H	1.70	0.57
1:J:172:PRO:O	1:J:173:HIS:HB2	2.04	0.57
1:I:192:ILE:O	1:I:195:GLU:HG3	2.04	0.57
1:J:362:TYR:HA	1:J:369:ILE:HG21	1.86	0.57
1:A:21:PHE:HB2	1:A:24:ASP:OD2	2.03	0.57
1:G:144:ALA:HB2	1:G:342:GLY:HA2	1.85	0.57
1:G:291:LYS:HG2	1:G:292:ASP:N	2.19	0.57
1:I:109:PRO:HB2	1:I:161:HIS:CE1	2.40	0.57
1:J:282:ILE:CG2	1:J:290:ARG:HG2	2.35	0.57
1:B:136:ILE:O	1:B:140:LEU:HD13	2.04	0.57
1:D:286:ASP:HB3	1:D:289:ILE:HD12	1.85	0.57
1:E:223:PHE:HB2	1:E:259:GLU:CD	2.25	0.57
1:A:37:ARG:O	1:A:66:THR:HG23	2.04	0.57
1:F:43:VAL:HG13	1:F:44:MET:N	2.20	0.57
1:F:99:GLU:HA	1:F:128:ASN:O	2.04	0.57
1:D:28:ARG:HG2	1:D:94:LEU:HD23	1.87	0.57
1:G:189:LEU:O	1:G:193:LEU:HD13	2.04	0.57
1:I:25:ASP:O	1:I:340:TRP:HZ3	1.87	0.56
1:G:104:LEU:CD2	1:G:347:ALA:HB2	2.35	0.56
1:A:142:LEU:HG	1:A:147:ARG:O	2.05	0.56
1:B:8:LEU:HB3	1:B:102:PRO:O	2.05	0.56
1:E:353:GLN:HA	1:E:356:TRP:CE2	2.40	0.56
1:F:54:VAL:HG21	1:F:85:ILE:HA	1.87	0.56
1:G:23:GLY:HA2	1:G:348:SER:HB3	1.87	0.56
1:G:282:ILE:CG2	1:G:290:ARG:HG2	2.35	0.56
1:I:35:VAL:HG21	1:I:81:ASP:HB2	1.86	0.56
1:I:230:ALA:HA	1:I:236:LEU:CD2	2.35	0.56
1:I:252:ASN:HA	1:I:255:PHE:CE2	2.41	0.56
1:D:136:ILE:HG21	1:D:375:PHE:CZ	2.40	0.56
1:D:151:ILE:HG22	1:D:297:ASN:HD22	1.69	0.56
1:G:110:LEU:O	1:G:110:LEU:HD22	2.05	0.56
1:J:282:ILE:HA	1:J:285:CYS:SG	2.45	0.56
1:C:136:ILE:HD12	1:C:169:TYR:CD2	2.40	0.56
1:G:4:GLU:HG3	1:G:5:THR:N	2.20	0.56
1:J:295:ALA:O	1:J:328:LYS:HB3	2.06	0.56
1:A:157:ASP:OD2	1:A:183:ARG:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ALA:HA	1:D:236:LEU:HD22	1.86	0.56
1:I:362:TYR:CD1	1:I:369:ILE:HG21	2.40	0.56
1:A:142:LEU:HD22	1:A:165:ILE:HG21	1.88	0.56
1:C:21:PHE:HB2	1:C:24:ASP:OD2	2.06	0.56
1:F:142:LEU:HD22	1:F:165:ILE:CG2	2.35	0.56
1:G:285:CYS:O	1:G:286:ASP:HB2	2.06	0.56
1:A:151:ILE:HD12	1:A:164:PRO:HA	1.88	0.56
1:C:54:VAL:HG21	1:C:85:ILE:HA	1.88	0.56
1:E:137:GLN:HG3	1:E:339:VAL:CG1	2.35	0.56
1:F:124:PHE:CD2	1:F:359:LYS:HD3	2.41	0.56
1:G:151:ILE:CG2	1:G:297:ASN:HD22	2.19	0.56
1:G:257:CYS:HB3	1:G:258:PRO:HD3	1.87	0.56
1:I:357:ILE:CD1	1:I:373:LYS:HG3	2.36	0.56
1:C:279:TYR:OH	1:C:317:ILE:HA	2.06	0.56
1:E:219:VAL:HG22	1:E:258:PRO:HB3	1.88	0.56
1:H:264:PRO:HG2	1:H:272:ALA:C	2.27	0.56
1:I:189:LEU:O	1:I:193:LEU:HD13	2.06	0.56
1:A:178:LEU:HG	1:A:180:LEU:H	1.71	0.55
1:A:299:MET:HB3	1:A:304:THR:HG21	1.87	0.55
1:H:124:PHE:CD2	1:H:359:LYS:HB2	2.41	0.55
1:G:327:ILE:N	1:G:327:ILE:CD1	2.69	0.55
1:I:121:GLN:HG3	1:I:125:GLU:OE1	2.06	0.55
1:A:12:ASN:HD21	1:A:71:ILE:HD11	1.71	0.55
1:C:279:TYR:O	1:C:283:MET:HG2	2.07	0.55
1:E:111:ASN:HB3	1:E:116:ARG:HH12	1.71	0.55
1:E:171:LEU:HA	1:E:375:PHE:CB	2.36	0.55
1:E:220:ALA:O	1:E:312:ARG:HD2	2.06	0.55
1:H:345:ILE:O	1:H:345:ILE:HG22	2.06	0.55
1:E:5:THR:HG21	1:E:356:TRP:CZ2	2.42	0.55
1:J:147:ARG:HH21	1:J:296:ASN:HD21	1.53	0.55
1:F:219:VAL:HG12	1:F:312:ARG:HD2	1.89	0.55
1:D:37:ARG:O	1:D:66:THR:HG23	2.06	0.55
1:E:49:GLN:O	1:E:50:LYS:HG2	2.07	0.55
1:E:99:GLU:O	1:E:130:PRO:HD3	2.07	0.55
1:E:172:PRO:HD3	1:E:375:PHE:HB2	1.87	0.55
1:J:6:THR:HG22	1:J:7:ALA:H	1.69	0.55
1:I:73:HIS:CE1	1:I:183:ARG:HE	2.24	0.55
1:J:73:HIS:HA	1:J:159:VAL:HG13	1.88	0.55
1:J:213:LYS:HA	1:J:217:CYS:SG	2.47	0.55
1:A:189:LEU:HD23	1:A:209:VAL:HG13	1.87	0.55
1:B:185:LEU:HB3	1:B:257:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LEU:HD13	1:E:119:MET:SD	2.47	0.55
1:F:242:LEU:HD23	1:F:244:ASP:H	1.71	0.55
1:H:136:ILE:HD13	1:H:375:PHE:CE1	2.42	0.55
1:D:211:ASP:O	1:D:215:LYS:HG2	2.07	0.55
1:D:213:LYS:HA	1:D:217:CYS:SG	2.46	0.55
1:G:110:LEU:HD11	1:G:161:HIS:NE2	2.22	0.55
1:D:289:ILE:HG22	1:D:293:LEU:CG	2.37	0.55
1:G:135:ALA:HB1	1:G:140:LEU:HD11	1.88	0.55
1:H:167:GLU:HG2	1:H:167:GLU:O	2.07	0.55
1:H:294:TYR:HB3	1:H:327:ILE:HD13	1.89	0.55
1:I:8:LEU:O	1:I:104:LEU:HB3	2.07	0.55
1:D:279:TYR:OH	1:D:317:ILE:HA	2.06	0.54
1:F:32:PRO:HG3	1:F:59:GLN:OE1	2.07	0.54
1:I:151:ILE:CD1	1:I:164:PRO:HA	2.37	0.54
1:J:287:ILE:HD13	1:J:290:ARG:NH1	2.20	0.54
1:A:189:LEU:O	1:A:193:LEU:HD13	2.07	0.54
1:D:220:ALA:O	1:D:312:ARG:HD2	2.08	0.54
1:I:142:LEU:HD22	1:I:165:ILE:CG2	2.37	0.54
1:J:185:LEU:HD11	1:J:261:LEU:HD11	1.90	0.54
1:H:73:HIS:HA	1:H:159:VAL:HG23	1.88	0.54
1:I:197:GLY:HA2	1:J:113:LYS:HB2	1.89	0.54
1:I:337:TYR:O	1:I:341:ILE:HG12	2.08	0.54
1:J:183:ARG:HG3	1:J:184:ASP:N	2.22	0.54
1:H:7:ALA:O	1:H:22:ALA:HB2	2.07	0.54
1:I:61:LYS:O	1:I:65:LEU:HD13	2.08	0.54
1:A:117:GLU:OE1	1:A:367:PRO:HA	2.07	0.54
1:F:164:PRO:HG3	1:F:174:ALA:CB	2.37	0.54
1:G:9:VAL:O	1:G:19:ALA:HA	2.06	0.54
1:G:90:PHE:HA	1:G:94:LEU:HD12	1.89	0.54
1:G:104:LEU:HD22	1:G:347:ALA:HB2	1.90	0.54
1:G:286:ASP:CB	1:G:289:ILE:HD12	2.38	0.54
1:B:27:PRO:HD3	1:B:340:TRP:CH2	2.43	0.54
1:C:144:ALA:HA	1:C:345:ILE:HD12	1.88	0.54
1:I:31:PHE:HE2	1:I:85:ILE:HG23	1.73	0.54
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.89	0.54
1:A:133:TYR:CE1	1:A:356:TRP:HA	2.43	0.54
1:B:133:TYR:CE1	1:B:356:TRP:HA	2.43	0.54
1:C:136:ILE:HD12	1:C:169:TYR:HD2	1.72	0.54
1:E:188:TYR:CD1	1:E:267:ILE:HG22	2.41	0.54
1:H:116:ARG:HD3	1:H:370:VAL:CG1	2.37	0.54
1:J:12:ASN:H	1:J:106:THR:HG22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:PHE:O	1:J:94:LEU:HB2	2.08	0.54
1:C:180:LEU:HD21	1:C:261:LEU:CA	2.30	0.54
1:D:71:ILE:HG12	1:D:76:ILE:HG12	1.89	0.54
1:D:140:LEU:HB3	1:D:342:GLY:HA3	1.90	0.54
1:D:276:GLU:HA	1:D:279:TYR:CD1	2.42	0.54
1:D:285:CYS:O	1:D:286:ASP:HB2	2.07	0.54
1:H:8:LEU:HD21	1:H:90:PHE:HE1	1.71	0.54
1:J:165:ILE:HG12	1:J:167:GLU:H	1.73	0.54
1:J:365:ALA:HB3	1:J:369:ILE:HD13	1.90	0.54
1:D:48:GLY:O	1:D:49:GLN:HB2	2.08	0.54
1:I:124:PHE:CE1	1:I:132:MET:HG2	2.43	0.54
1:B:6:THR:O	1:B:7:ALA:HB2	2.07	0.54
1:D:47:MET:HG3	1:D:48:GLY:N	2.23	0.54
1:E:171:LEU:HA	1:E:375:PHE:HB2	1.90	0.54
1:H:116:ARG:HH11	1:H:116:ARG:HG3	1.71	0.54
1:I:90:PHE:HA	1:I:94:LEU:HD12	1.90	0.54
1:E:64:ILE:HD12	1:G:288:ASP:HB2	1.89	0.53
1:E:340:TRP:CE3	1:E:341:ILE:HD13	2.43	0.53
1:I:151:ILE:CG2	1:I:297:ASN:HD22	2.21	0.53
1:D:158:GLY:O	1:D:159:VAL:HG13	2.08	0.53
1:F:39:ARG:HD2	1:F:63:GLY:O	2.08	0.53
1:J:124:PHE:CE1	1:J:132:MET:HG2	2.43	0.53
1:C:110:LEU:HD12	1:C:177:ARG:HG3	1.89	0.53
1:E:230:ALA:HA	1:E:236:LEU:HD22	1.91	0.53
1:I:200:PHE:HB3	1:I:205:GLU:HG3	1.89	0.53
1:J:121:GLN:HG3	1:J:125:GLU:OE1	2.09	0.53
1:J:230:ALA:HA	1:J:236:LEU:CD2	2.35	0.53
1:J:287:ILE:HA	1:J:290:ARG:HH11	1.73	0.53
1:D:9:VAL:O	1:D:19:ALA:HA	2.07	0.53
1:F:137:GLN:HG3	1:F:339:VAL:CG1	2.38	0.53
1:G:164:PRO:HG3	1:G:174:ALA:CB	2.38	0.53
1:D:208:ILE:HG21	1:D:242:LEU:HD11	1.89	0.53
1:C:276:GLU:HA	1:C:279:TYR:CD1	2.44	0.53
1:D:121:GLN:HG3	1:D:125:GLU:OE1	2.09	0.53
1:F:276:GLU:HA	1:F:279:TYR:CD1	2.44	0.53
1:G:109:PRO:C	1:G:110:LEU:HD13	2.28	0.53
1:G:223:PHE:CD1	1:G:259:GLU:HG2	2.44	0.53
1:H:104:LEU:HD22	1:H:347:ALA:CB	2.37	0.53
1:H:136:ILE:HD12	1:H:169:TYR:HD2	1.73	0.53
1:I:220:ALA:HB1	1:I:226:GLU:OE2	2.09	0.53
1:J:289:ILE:O	1:J:293:LEU:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PRO:HB2	1:C:161:HIS:CE1	2.44	0.53
1:E:178:LEU:HG	1:E:180:LEU:H	1.73	0.53
1:A:172:PRO:O	1:A:173:HIS:HB2	2.08	0.53
1:G:63:GLY:HA3	1:I:287:ILE:CG2	2.33	0.53
1:G:223:PHE:HB2	1:G:259:GLU:CD	2.30	0.53
1:H:189:LEU:HD23	1:H:209:VAL:HG13	1.91	0.53
1:H:346:LEU:HD22	1:H:352:PHE:CD1	2.44	0.53
1:J:257:CYS:HB3	1:J:258:PRO:HD3	1.89	0.53
1:C:8:LEU:HD12	1:C:20:GLY:O	2.08	0.53
1:C:103:THR:O	1:C:132:MET:HA	2.09	0.53
1:D:252:ASN:HA	1:D:255:PHE:CE2	2.44	0.53
1:F:189:LEU:HD23	1:F:209:VAL:HG13	1.89	0.53
1:G:133:TYR:CE1	1:G:356:TRP:HA	2.44	0.53
1:G:151:ILE:HG22	1:G:297:ASN:HD22	1.74	0.53
1:H:21:PHE:HB2	1:H:24:ASP:OD2	2.09	0.53
1:B:37:ARG:HG3	1:B:38:PRO:HD2	1.91	0.53
1:B:279:TYR:OH	1:B:317:ILE:HA	2.08	0.53
1:D:70:PRO:O	1:D:76:ILE:HA	2.09	0.53
1:E:6:THR:CG2	1:E:22:ALA:HB3	2.37	0.53
1:F:20:GLY:HA2	1:F:94:LEU:HD21	1.91	0.53
1:G:276:GLU:HA	1:G:279:TYR:CD1	2.43	0.53
1:I:172:PRO:O	1:I:173:HIS:HB2	2.09	0.53
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.91	0.52
1:I:12:ASN:H	1:I:106:THR:HG22	1.74	0.52
1:I:110:LEU:HD12	1:I:177:ARG:HB2	1.90	0.52
1:I:189:LEU:HD23	1:I:209:VAL:HG13	1.91	0.52
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.90	0.52
1:G:272:ALA:HB3	1:G:276:GLU:HB2	1.90	0.52
1:J:284:LYS:HB2	1:J:284:LYS:HZ2	1.75	0.52
1:E:291:LYS:HG2	1:E:292:ASP:N	2.24	0.52
1:F:5:THR:C	1:F:102:PRO:HG2	2.29	0.52
1:A:256:ARG:O	1:A:259:GLU:HB3	2.09	0.52
1:D:289:ILE:HG22	1:D:293:LEU:HG	1.91	0.52
1:H:111:ASN:HB3	1:H:116:ARG:HH12	1.74	0.52
1:I:213:LYS:O	1:I:217:CYS:HB2	2.10	0.52
1:I:236:LEU:HA	1:I:254:ARG:HH21	1.74	0.52
1:J:220:ALA:HB1	1:J:226:GLU:OE2	2.10	0.52
1:G:140:LEU:HG	1:G:346:LEU:HD12	1.92	0.52
1:G:180:LEU:CD2	1:G:261:LEU:HA	2.37	0.52
1:G:255:PHE:C	1:G:258:PRO:HD2	2.30	0.52
1:J:11:ASP:HB3	1:J:18:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:C	1:A:258:PRO:HD2	2.30	0.52
1:F:6:THR:O	1:F:7:ALA:HB2	2.10	0.52
1:G:327:ILE:H	1:G:327:ILE:CD1	2.22	0.52
1:I:188:TYR:HD2	1:I:257:CYS:SG	2.33	0.52
1:J:164:PRO:HG3	1:J:285:CYS:SG	2.49	0.52
1:J:281:SER:HA	1:J:284:LYS:NZ	2.24	0.52
1:E:283:MET:HG2	1:E:290:ARG:NH2	2.25	0.52
1:F:171:LEU:HD12	1:F:171:LEU:H	1.74	0.52
1:H:110:LEU:HD13	1:H:177:ARG:HB2	1.92	0.52
1:H:116:ARG:HB3	1:H:370:VAL:HG21	1.92	0.52
1:I:219:VAL:HG23	1:I:306:TYR:HB2	1.91	0.52
1:A:287:ILE:HD13	1:A:290:ARG:NH1	2.24	0.52
1:I:202:THR:HG23	1:J:177:ARG:NH2	2.25	0.52
1:A:103:THR:O	1:A:132:MET:HA	2.10	0.52
1:D:140:LEU:HD23	1:D:343:GLY:HA2	1.91	0.52
1:F:116:ARG:HG2	1:F:370:VAL:HG11	1.91	0.52
1:H:299:MET:HB3	1:H:304:THR:CG2	2.35	0.52
1:J:293:LEU:HD12	1:J:293:LEU:C	2.30	0.52
1:B:286:ASP:HB3	1:B:289:ILE:HD12	1.92	0.52
1:F:12:ASN:HB3	1:F:71:ILE:HD13	1.92	0.52
1:G:167:GLU:O	1:G:167:GLU:HG2	2.10	0.52
1:F:169:TYR:HE1	1:F:355:MET:SD	2.32	0.51
1:H:230:ALA:HA	1:H:236:LEU:CD2	2.41	0.51
1:I:357:ILE:HD11	1:I:373:LYS:HG3	1.91	0.51
1:B:243:PRO:O	1:B:244:ASP:HB2	2.09	0.51
1:B:342:GLY:O	1:B:346:LEU:HG	2.11	0.51
1:E:9:VAL:HG22	1:E:104:LEU:HB3	1.93	0.51
1:F:5:THR:HB	1:F:102:PRO:CG	2.41	0.51
1:G:289:ILE:O	1:G:293:LEU:HG	2.11	0.51
1:I:167:GLU:O	1:I:167:GLU:HG2	2.11	0.51
1:J:283:MET:HA	1:J:290:ARG:HH21	1.74	0.51
1:C:365:ALA:HB3	1:C:369:ILE:HD13	1.93	0.51
1:I:8:LEU:HD23	1:I:102:PRO:O	2.11	0.51
1:B:41:GLN:C	1:B:43:VAL:H	2.13	0.51
1:B:163:VAL:HG11	1:B:375:PHE:CZ	2.46	0.51
1:C:172:PRO:HD3	1:C:375:PHE:HB2	1.93	0.51
1:D:22:ALA:HB1	1:D:347:ALA:HB1	1.92	0.51
1:H:63:GLY:N	1:J:287:ILE:HB	2.26	0.51
1:F:109:PRO:HB2	1:F:161:HIS:CE1	2.45	0.51
1:H:270:GLU:HG3	1:H:271:SER:H	1.75	0.51
1:H:294:TYR:HB3	1:H:327:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:LEU:HG	1:I:180:LEU:H	1.75	0.51
1:I:242:LEU:HD22	1:I:244:ASP:HB3	1.92	0.51
1:A:180:LEU:HD21	1:A:261:LEU:HA	1.92	0.51
1:A:181:ALA:O	1:A:184:ASP:HB2	2.10	0.51
1:F:94:LEU:HB3	1:F:96:VAL:HG22	1.92	0.51
1:H:61:LYS:HB2	1:H:61:LYS:NZ	2.26	0.51
1:H:314:GLN:HE22	1:H:328:LYS:HA	1.75	0.51
1:C:223:PHE:HB2	1:C:259:GLU:CD	2.30	0.51
1:D:286:ASP:HB3	1:D:289:ILE:CD1	2.41	0.51
1:H:252:ASN:HA	1:H:255:PHE:CE2	2.46	0.51
1:H:116:ARG:HH11	1:H:116:ARG:HG2	1.76	0.51
1:A:105:LEU:HD13	1:A:119:MET:SD	2.50	0.50
1:C:151:ILE:CG1	1:C:293:LEU:HD22	2.41	0.50
1:D:248:ILE:HG22	1:D:250:ILE:HG23	1.92	0.50
1:E:71:ILE:HD13	1:E:76:ILE:HG12	1.93	0.50
1:F:43:VAL:HG22	1:F:44:MET:H	1.77	0.50
1:F:219:VAL:HG22	1:F:258:PRO:HB3	1.92	0.50
1:G:54:VAL:HG23	1:G:85:ILE:HD13	1.92	0.50
1:J:193:LEU:HB3	1:J:198:TYR:O	2.11	0.50
1:C:140:LEU:HG	1:C:346:LEU:HD12	1.92	0.50
1:C:161:HIS:NE2	1:C:177:ARG:HG2	2.25	0.50
1:D:8:LEU:HD12	1:D:20:GLY:O	2.11	0.50
1:I:289:ILE:O	1:I:293:LEU:HG	2.11	0.50
1:J:236:LEU:HA	1:J:254:ARG:HH21	1.77	0.50
1:J:252:ASN:HA	1:J:255:PHE:CE2	2.46	0.50
1:F:166:TYR:CE1	1:F:289:ILE:HD13	2.47	0.50
1:H:213:LYS:HA	1:H:217:CYS:SG	2.50	0.50
1:D:140:LEU:HD23	1:D:343:GLY:CA	2.41	0.50
1:D:189:LEU:HD23	1:D:209:VAL:HG13	1.92	0.50
1:H:61:LYS:HA	1:J:291:LYS:HD2	1.94	0.50
1:A:58:ALA:HB1	1:A:65:LEU:CD2	2.37	0.50
1:B:124:PHE:CZ	1:B:359:LYS:HB2	2.47	0.50
1:B:180:LEU:HD11	1:B:267:ILE:CD1	2.41	0.50
1:J:189:LEU:O	1:J:193:LEU:HD13	2.11	0.50
1:E:139:VAL:HG11	1:E:169:TYR:CE2	2.47	0.50
1:I:71:ILE:HG12	1:I:76:ILE:HG12	1.94	0.50
1:J:314:GLN:OE1	1:J:329:ILE:HG12	2.12	0.50
1:F:63:GLY:HA3	1:H:287:ILE:HB	1.94	0.50
1:H:178:LEU:HG	1:H:180:LEU:H	1.76	0.50
1:H:306:TYR:HD1	1:H:306:TYR:H	1.60	0.50
1:I:198:TYR:CZ	1:I:248:ILE:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:GLY:HA2	1:J:293:LEU:HA	1.93	0.50
1:A:287:ILE:HA	1:A:290:ARG:HH12	1.74	0.50
1:C:144:ALA:HA	1:C:345:ILE:CD1	2.42	0.50
1:D:103:THR:O	1:D:132:MET:HB2	2.11	0.50
1:E:136:ILE:O	1:E:140:LEU:HD13	2.12	0.50
1:A:123:MET:SD	1:A:132:MET:SD	3.10	0.50
1:B:189:LEU:HD23	1:B:209:VAL:HG13	1.94	0.50
1:B:236:LEU:HA	1:B:254:ARG:HH21	1.76	0.50
1:C:358:THR:HG22	1:C:359:LYS:H	1.76	0.50
1:D:149:THR:HB	1:D:292:ASP:OD1	2.11	0.50
1:D:223:PHE:CD1	1:D:259:GLU:HG2	2.46	0.50
1:D:299:MET:HB3	1:D:304:THR:HG21	1.93	0.50
1:E:110:LEU:HD21	1:E:175:ILE:HD11	1.94	0.50
1:I:213:LYS:HD2	1:I:306:TYR:OH	2.12	0.50
1:A:337:TYR:O	1:A:341:ILE:HG13	2.12	0.49
1:B:136:ILE:HD11	1:B:374:CYS:CB	2.42	0.49
1:C:14:SER:HB2	1:C:157:ASP:HB3	1.94	0.49
1:C:196:ARG:O	1:C:196:ARG:HD3	2.12	0.49
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.94	0.49
1:A:291:LYS:H	1:A:291:LYS:HD2	1.77	0.49
1:B:255:PHE:C	1:B:258:PRO:HD2	2.32	0.49
1:C:135:ALA:HB1	1:C:140:LEU:HD11	1.94	0.49
1:D:283:MET:HG2	1:D:290:ARG:NH2	2.27	0.49
1:J:35:VAL:HG21	1:J:81:ASP:HB2	1.94	0.49
1:J:281:SER:HA	1:J:284:LYS:HZ2	1.78	0.49
1:B:180:LEU:HD11	1:B:267:ILE:HD13	1.94	0.49
1:B:223:PHE:HB2	1:B:259:GLU:CD	2.33	0.49
1:E:109:PRO:HB2	1:E:161:HIS:CE1	2.48	0.49
1:H:346:LEU:HD13	1:H:352:PHE:CE1	2.48	0.49
1:J:279:TYR:CE1	1:J:320:LEU:HB2	2.47	0.49
1:B:172:PRO:O	1:B:173:HIS:HB2	2.12	0.49
1:E:140:LEU:CD1	1:E:346:LEU:HD11	2.42	0.49
1:I:164:PRO:HD2	1:I:175:ILE:HG22	1.95	0.49
1:J:216:LEU:HD22	1:J:238:LYS:HD2	1.93	0.49
1:J:221:LEU:HD11	1:J:315:LYS:HD3	1.95	0.49
1:A:111:ASN:HB3	1:A:116:ARG:HH12	1.76	0.49
1:D:147:ARG:HH21	1:D:296:ASN:HD21	1.61	0.49
1:F:104:LEU:HD22	1:F:347:ALA:HB2	1.93	0.49
1:G:220:ALA:O	1:G:312:ARG:HD2	2.12	0.49
1:H:155:SER:OG	1:H:160:THR:HA	2.13	0.49
1:I:188:TYR:CE1	1:I:267:ILE:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LYS:HA	1:C:217:CYS:SG	2.53	0.49
1:G:63:GLY:HA2	1:I:287:ILE:HD13	1.95	0.49
1:C:230:ALA:HA	1:C:236:LEU:HD22	1.95	0.49
1:E:47:MET:HA	1:G:166:TYR:CE2	2.48	0.49
1:F:213:LYS:HA	1:F:217:CYS:SG	2.52	0.49
1:J:255:PHE:C	1:J:258:PRO:HD2	2.33	0.49
1:B:286:ASP:HB3	1:B:289:ILE:CD1	2.43	0.49
1:B:286:ASP:O	1:B:289:ILE:HB	2.12	0.49
1:A:63:GLY:CA	1:C:287:ILE:HG21	2.24	0.49
1:E:8:LEU:HB3	1:E:102:PRO:O	2.12	0.49
1:E:140:LEU:HG	1:E:346:LEU:HD11	1.94	0.49
1:F:133:TYR:HD1	1:F:357:ILE:H	1.60	0.49
1:C:8:LEU:HB3	1:C:103:THR:HA	1.95	0.48
1:D:149:THR:OG1	1:D:292:ASP:HB2	2.13	0.48
1:D:219:VAL:HG22	1:D:258:PRO:CB	2.42	0.48
1:F:179:ASP:OD2	1:F:269:MET:HE1	2.13	0.48
1:I:144:ALA:HA	1:I:345:ILE:HG13	1.95	0.48
1:A:120:THR:HG23	1:A:124:PHE:CE1	2.48	0.48
1:E:38:PRO:HG3	1:E:44:MET:SD	2.53	0.48
1:G:17:VAL:HG23	1:G:33:SER:HB2	1.94	0.48
1:G:331:ALA:HB1	1:G:335:ARG:HH11	1.79	0.48
1:A:140:LEU:HG	1:A:346:LEU:HD11	1.95	0.48
1:A:353:GLN:HA	1:A:356:TRP:CE2	2.48	0.48
1:B:151:ILE:HD12	1:B:164:PRO:CA	2.43	0.48
1:B:260:THR:HG23	1:B:267:ILE:HG21	1.95	0.48
1:C:70:PRO:O	1:C:76:ILE:HG23	2.12	0.48
1:E:270:GLU:HG2	1:E:271:SER:N	2.28	0.48
1:F:188:TYR:CE1	1:F:267:ILE:HG22	2.48	0.48
1:F:314:GLN:OE1	1:F:329:ILE:HG12	2.13	0.48
1:I:151:ILE:HD12	1:I:164:PRO:HA	1.95	0.48
1:I:197:GLY:HA2	1:J:113:LYS:CG	2.42	0.48
1:J:39:ARG:HD2	1:J:63:GLY:O	2.13	0.48
1:J:372:ARG:CZ	1:J:372:ARG:HA	2.44	0.48
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.95	0.48
1:C:41:GLN:HG2	1:C:43:VAL:N	2.28	0.48
1:C:133:TYR:CE1	1:C:356:TRP:HA	2.48	0.48
1:C:236:LEU:HA	1:C:254:ARG:HH21	1.77	0.48
1:E:172:PRO:O	1:E:173:HIS:HB2	2.13	0.48
1:H:353:GLN:HG3	1:H:356:TRP:CZ2	2.48	0.48
1:I:157:ASP:OD2	1:I:183:ARG:HB3	2.14	0.48
1:I:193:LEU:HB3	1:I:198:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:THR:HG22	1:J:282:ILE:HD12	1.96	0.48
1:A:14:SER:CB	1:A:157:ASP:HB3	2.44	0.48
1:F:172:PRO:O	1:F:173:HIS:CB	2.62	0.48
1:G:10:CYS:HA	1:G:18:LYS:O	2.13	0.48
1:H:31:PHE:HZ	1:H:89:THR:HG1	1.59	0.48
1:B:142:LEU:HD22	1:B:165:ILE:HG21	1.96	0.48
1:C:136:ILE:HD13	1:C:375:PHE:HE1	1.75	0.48
1:E:28:ARG:HB2	1:E:94:LEU:HD23	1.96	0.48
1:F:183:ARG:HH11	1:F:183:ARG:HB2	1.79	0.48
1:G:23:GLY:HA2	1:G:348:SER:CB	2.44	0.48
1:H:172:PRO:O	1:H:173:HIS:HB2	2.14	0.48
1:I:223:PHE:HB2	1:I:259:GLU:CD	2.34	0.48
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.49	0.48
1:B:260:THR:CG2	1:B:267:ILE:HG21	2.44	0.48
1:C:189:LEU:O	1:C:193:LEU:HD13	2.13	0.48
1:F:211:ASP:O	1:F:215:LYS:HG2	2.13	0.48
1:G:213:LYS:HA	1:G:217:CYS:SG	2.54	0.48
1:I:304:THR:O	1:I:309:ILE:HG21	2.14	0.48
1:J:151:ILE:CG2	1:J:293:LEU:HD13	2.44	0.48
1:D:243:PRO:O	1:D:244:ASP:HB2	2.13	0.48
1:F:147:ARG:HE	1:F:296:ASN:ND2	2.12	0.48
1:G:166:TYR:CE1	1:G:289:ILE:HG12	2.48	0.48
1:I:155:SER:O	1:I:301:GLY:HA3	2.14	0.48
1:J:301:GLY:O	1:J:305:MET:HG2	2.14	0.48
1:B:178:LEU:HG	1:B:180:LEU:H	1.79	0.48
1:E:171:LEU:HA	1:E:375:PHE:CG	2.49	0.48
1:G:20:GLY:HA2	1:G:94:LEU:CD2	2.43	0.48
1:I:219:VAL:HG22	1:I:258:PRO:CB	2.43	0.48
1:I:305:MET:SD	1:I:336:LYS:HB2	2.54	0.48
1:J:192:ILE:HG21	1:J:256:ARG:HD2	1.95	0.48
1:J:290:ARG:HA	1:J:293:LEU:CD2	2.43	0.48
1:D:272:ALA:HB3	1:D:276:GLU:HB2	1.95	0.47
1:D:305:MET:HE3	1:D:336:LYS:HD2	1.96	0.47
1:H:61:LYS:HB3	1:J:288:ASP:CB	2.44	0.47
1:J:345:ILE:O	1:J:349:LEU:HG	2.14	0.47
1:B:267:ILE:HG13	1:B:268:GLY:N	2.29	0.47
1:D:61:LYS:HB2	1:D:61:LYS:NZ	2.29	0.47
1:D:183:ARG:HG3	1:D:184:ASP:N	2.29	0.47
1:H:345:ILE:HG23	1:H:349:LEU:HD12	1.96	0.47
1:J:113:LYS:HA	1:J:116:ARG:HD3	1.96	0.47
1:B:166:TYR:CG	1:B:167:GLU:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:TYR:CD2	1:H:352:PHE:HZ	2.32	0.47
1:I:282:ILE:CG2	1:I:290:ARG:HG2	2.44	0.47
1:C:139:VAL:HG21	1:C:169:TYR:CD2	2.49	0.47
1:C:248:ILE:HG22	1:C:250:ILE:HG23	1.96	0.47
1:D:294:TYR:HB3	1:D:327:ILE:HD13	1.95	0.47
1:E:213:LYS:HA	1:E:217:CYS:SG	2.54	0.47
1:G:37:ARG:O	1:G:66:THR:HG23	2.13	0.47
1:G:279:TYR:OH	1:G:317:ILE:HA	2.14	0.47
1:H:61:LYS:O	1:J:288:ASP:HA	2.14	0.47
1:J:88:HIS:O	1:J:92:ASN:HB2	2.15	0.47
1:C:220:ALA:O	1:C:312:ARG:HD2	2.15	0.47
1:D:8:LEU:CB	1:D:102:PRO:O	2.63	0.47
1:D:39:ARG:HG3	1:D:40:HIS:H	1.80	0.47
1:E:122:ILE:O	1:E:126:THR:HB	2.14	0.47
1:G:151:ILE:CD1	1:G:164:PRO:HA	2.44	0.47
1:I:255:PHE:C	1:I:258:PRO:HD2	2.35	0.47
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.97	0.47
1:A:172:PRO:HD3	1:A:375:PHE:HB2	1.97	0.47
1:A:304:THR:HG22	1:A:309:ILE:HD12	1.97	0.47
1:A:314:GLN:OE1	1:A:329:ILE:HG12	2.14	0.47
1:E:236:LEU:HA	1:E:254:ARG:HH21	1.80	0.47
1:F:220:ALA:O	1:F:312:ARG:HD2	2.15	0.47
1:F:300:SER:HA	1:F:335:ARG:HB2	1.96	0.47
1:H:38:PRO:HA	1:H:64:ILE:HG23	1.97	0.47
1:H:192:ILE:HG21	1:H:256:ARG:HD2	1.95	0.47
1:I:36:GLY:HA2	1:I:66:THR:O	2.14	0.47
1:I:218:TYR:O	1:I:258:PRO:HG2	2.15	0.47
1:J:211:ASP:O	1:J:215:LYS:HG2	2.14	0.47
1:J:219:VAL:HG22	1:J:258:PRO:CB	2.44	0.47
1:J:279:TYR:O	1:J:283:MET:HG2	2.13	0.47
1:A:345:ILE:O	1:A:349:LEU:HG	2.15	0.47
1:D:289:ILE:HG22	1:D:293:LEU:HD11	1.96	0.47
1:F:252:ASN:HA	1:F:255:PHE:CE2	2.49	0.47
1:B:27:PRO:HD3	1:B:340:TRP:CZ2	2.50	0.47
1:B:110:LEU:HD12	1:B:161:HIS:CD2	2.50	0.47
1:B:289:ILE:HG22	1:B:293:LEU:CD1	2.40	0.47
1:D:192:ILE:HG21	1:D:256:ARG:HD2	1.96	0.47
1:F:167:GLU:O	1:F:167:GLU:HG2	2.15	0.47
1:F:299:MET:HB3	1:F:304:THR:HG21	1.96	0.47
1:G:150:GLY:O	1:G:165:ILE:HG21	2.15	0.47
1:G:230:ALA:HA	1:G:236:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:CG2	1:B:293:LEU:HD11	2.41	0.47
1:C:200:PHE:HZ	1:C:248:ILE:HD11	1.79	0.47
1:F:8:LEU:HD23	1:F:21:PHE:HA	1.97	0.47
1:F:61:LYS:HG2	1:H:291:LYS:CE	2.45	0.47
1:I:174:ALA:HB1	1:I:285:CYS:HA	1.96	0.47
1:J:135:ALA:HB1	1:J:140:LEU:HD11	1.97	0.47
1:A:124:PHE:CE1	1:A:132:MET:HB3	2.50	0.46
1:B:166:TYR:CD1	1:B:289:ILE:HG12	2.49	0.46
1:B:213:LYS:HA	1:B:217:CYS:SG	2.55	0.46
1:C:272:ALA:HB3	1:C:276:GLU:HB2	1.97	0.46
1:D:57:GLU:HG2	1:D:61:LYS:HE3	1.97	0.46
1:G:246:GLN:NE2	1:H:113:LYS:HE3	2.29	0.46
1:H:10:CYS:O	1:H:105:LEU:HA	2.15	0.46
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.97	0.46
1:D:53:TYR:HB2	1:D:65:LEU:CD2	2.44	0.46
1:H:257:CYS:O	1:H:260:THR:HB	2.15	0.46
1:I:270:GLU:HG2	1:I:271:SER:N	2.30	0.46
1:J:278:THR:HG22	1:J:282:ILE:CD1	2.45	0.46
1:A:9:VAL:O	1:A:19:ALA:HA	2.15	0.46
1:A:180:LEU:CD2	1:A:261:LEU:HA	2.46	0.46
1:A:286:ASP:HB3	1:A:289:ILE:CD1	2.42	0.46
1:C:121:GLN:HG3	1:C:125:GLU:OE1	2.16	0.46
1:D:123:MET:HB2	1:D:132:MET:SD	2.55	0.46
1:E:225:ASN:HD22	1:E:225:ASN:C	2.19	0.46
1:J:153:LEU:HG	1:J:162:ASN:ND2	2.30	0.46
1:B:6:THR:O	1:B:7:ALA:CB	2.62	0.46
1:B:10:CYS:HA	1:B:18:LYS:O	2.16	0.46
1:B:99:GLU:O	1:B:130:PRO:HD3	2.15	0.46
1:E:346:LEU:HD13	1:E:352:PHE:CZ	2.50	0.46
1:F:111:ASN:HB3	1:F:116:ARG:HH12	1.77	0.46
1:G:7:ALA:HB2	1:G:102:PRO:HB2	1.96	0.46
1:J:371:HIS:HA	1:J:374:CYS:O	2.16	0.46
1:A:23:GLY:HA2	1:A:348:SER:OG	2.15	0.46
1:C:169:TYR:HE1	1:C:355:MET:SD	2.39	0.46
1:C:283:MET:SD	1:C:290:ARG:NH2	2.89	0.46
1:D:151:ILE:CG2	1:D:297:ASN:HD22	2.27	0.46
1:E:180:LEU:CD2	1:E:261:LEU:HA	2.39	0.46
1:F:289:ILE:O	1:F:293:LEU:HG	2.16	0.46
1:H:306:TYR:N	1:H:306:TYR:CD1	2.84	0.46
1:I:216:LEU:HD22	1:I:238:LYS:HD2	1.96	0.46
1:G:24:ASP:O	1:G:25:ASP:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:GLU:HA	1:G:256:ARG:HB3	1.97	0.46
1:J:62:ARG:HE	1:J:207:GLU:CB	2.28	0.46
1:J:221:LEU:HD13	1:J:311:ASP:OD1	2.16	0.46
1:B:12:ASN:H	1:B:106:THR:HG22	1.80	0.46
1:B:300:SER:HA	1:B:335:ARG:HB2	1.98	0.46
1:F:8:LEU:CD2	1:F:21:PHE:HA	2.46	0.46
1:F:21:PHE:HB2	1:F:24:ASP:OD2	2.16	0.46
1:F:170:ALA:O	1:F:375:PHE:CD1	2.69	0.46
1:G:141:SER:OG	1:G:152:VAL:HG11	2.15	0.46
1:J:123:MET:O	1:J:127:PHE:O	2.34	0.46
1:C:223:PHE:CD1	1:C:259:GLU:HG2	2.51	0.46
1:C:337:TYR:O	1:C:341:ILE:HG12	2.15	0.46
1:D:155:SER:OG	1:D:160:THR:HA	2.15	0.46
1:E:110:LEU:HD12	1:E:177:ARG:HB2	1.97	0.46
1:E:142:LEU:HD22	1:E:165:ILE:HG23	1.98	0.46
1:E:189:LEU:HD23	1:E:209:VAL:HG13	1.97	0.46
1:F:163:VAL:HA	1:F:175:ILE:HG22	1.97	0.46
1:E:223:PHE:CD1	1:E:259:GLU:HG2	2.51	0.46
1:F:171:LEU:HD13	1:F:171:LEU:O	2.15	0.46
1:H:124:PHE:CE2	1:H:359:LYS:HB2	2.51	0.46
1:C:260:THR:CG2	1:C:267:ILE:HG21	2.46	0.46
1:D:7:ALA:HB1	1:D:104:LEU:HB2	1.98	0.46
1:D:10:CYS:HB3	1:D:105:LEU:CD2	2.46	0.46
1:D:172:PRO:O	1:D:173:HIS:HB3	2.16	0.46
1:E:35:VAL:HA	1:E:53:TYR:O	2.16	0.46
1:G:137:GLN:HG3	1:G:339:VAL:HG13	1.98	0.46
1:H:313:MET:HB2	1:H:329:ILE:HG13	1.98	0.46
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.97	0.46
1:A:219:VAL:HG22	1:A:258:PRO:HB3	1.97	0.45
1:C:11:ASP:O	1:C:17:VAL:HG13	2.16	0.45
1:D:47:MET:HG3	1:D:48:GLY:H	1.80	0.45
1:E:9:VAL:HG22	1:E:104:LEU:HD23	1.98	0.45
1:E:365:ALA:HB3	1:E:369:ILE:HD13	1.98	0.45
1:F:63:GLY:HA2	1:H:287:ILE:CD1	2.46	0.45
1:I:39:ARG:HB3	1:I:66:THR:CG2	2.47	0.45
1:C:260:THR:HG23	1:C:267:ILE:CG2	2.47	0.45
1:D:109:PRO:HB2	1:D:161:HIS:CE1	2.52	0.45
1:E:79:TRP:HZ2	1:E:115:ASN:ND2	2.14	0.45
1:E:255:PHE:C	1:E:258:PRO:HD2	2.36	0.45
1:F:183:ARG:HG3	1:F:184:ASP:N	2.30	0.45
1:G:103:THR:O	1:G:132:MET:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ILE:HG21	1:G:256:ARG:HD2	1.98	0.45
1:H:110:LEU:CD1	1:H:177:ARG:HB2	2.45	0.45
1:I:90:PHE:O	1:I:94:LEU:HB2	2.16	0.45
1:A:230:ALA:HA	1:A:236:LEU:CD2	2.47	0.45
1:C:172:PRO:HG3	1:C:375:PHE:HB2	1.98	0.45
1:D:171:LEU:CA	1:D:375:PHE:HB2	2.47	0.45
1:H:151:ILE:HG22	1:H:297:ASN:HD22	1.82	0.45
1:B:116:ARG:CG	1:B:370:VAL:HG21	2.43	0.45
1:D:304:THR:O	1:D:309:ILE:HG21	2.16	0.45
1:E:29:ALA:HB2	1:E:93:GLU:HG2	1.97	0.45
1:F:110:LEU:CD1	1:F:177:ARG:HB2	2.46	0.45
1:G:79:TRP:HZ2	1:G:115:ASN:ND2	2.14	0.45
1:J:208:ILE:HG21	1:J:242:LEU:HD11	1.99	0.45
1:A:208:ILE:HG21	1:A:242:LEU:HD11	1.98	0.45
1:E:6:THR:O	1:E:7:ALA:HB3	2.16	0.45
1:H:9:VAL:HA	1:H:104:LEU:HB3	1.97	0.45
1:I:99:GLU:O	1:I:130:PRO:HD3	2.16	0.45
1:I:346:LEU:HD21	1:I:352:PHE:CD1	2.52	0.45
1:J:226:GLU:O	1:J:229:THR:HB	2.16	0.45
1:D:151:ILE:HB	1:D:293:LEU:HD22	1.97	0.45
1:E:28:ARG:HB2	1:E:94:LEU:CD2	2.47	0.45
1:J:189:LEU:HD23	1:J:209:VAL:HG13	1.99	0.45
1:B:9:VAL:O	1:B:19:ALA:HA	2.17	0.45
1:B:29:ALA:HB2	1:B:93:GLU:CB	2.47	0.45
1:B:154:ASP:OD2	1:B:339:VAL:HG22	2.17	0.45
1:C:252:ASN:HA	1:C:255:PHE:CE2	2.52	0.45
1:D:164:PRO:HD2	1:D:175:ILE:HG22	1.98	0.45
1:F:250:ILE:HD12	1:F:254:ARG:CG	2.42	0.45
1:G:250:ILE:HG13	1:G:250:ILE:O	2.16	0.45
1:G:286:ASP:HB3	1:G:289:ILE:CD1	2.44	0.45
1:H:151:ILE:CG2	1:H:297:ASN:HD22	2.29	0.45
1:J:39:ARG:HG3	1:J:64:ILE:O	2.16	0.45
1:A:94:LEU:HB3	1:A:96:VAL:HG22	1.99	0.45
1:D:169:TYR:HE1	1:D:355:MET:SD	2.40	0.45
1:E:110:LEU:CD1	1:E:177:ARG:HB2	2.47	0.45
1:H:63:GLY:H	1:J:287:ILE:HB	1.81	0.45
1:I:352:PHE:CE2	1:I:356:TRP:HE3	2.35	0.45
1:J:111:ASN:HB3	1:J:116:ARG:HH12	1.81	0.45
1:J:299:MET:HB3	1:J:304:THR:HG21	1.97	0.45
1:A:5:THR:HA	1:A:102:PRO:HG2	1.99	0.45
1:A:289:ILE:HG22	1:A:293:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:THR:O	1:E:7:ALA:N	2.49	0.45
1:E:340:TRP:HE3	1:E:341:ILE:HD13	1.81	0.45
1:F:12:ASN:H	1:F:106:THR:HG22	1.82	0.45
1:G:63:GLY:CA	1:I:287:ILE:HG21	2.38	0.45
1:G:64:ILE:HD11	1:I:288:ASP:OD2	2.17	0.45
1:G:164:PRO:HG3	1:G:174:ALA:HB1	1.98	0.45
1:H:346:LEU:HD23	1:H:346:LEU:HA	1.81	0.45
1:I:200:PHE:CB	1:I:205:GLU:HG3	2.47	0.45
1:A:84:LYS:O	1:A:87:HIS:HB3	2.16	0.45
1:D:124:PHE:CZ	1:D:132:MET:HG2	2.49	0.45
1:F:306:TYR:N	1:F:306:TYR:CD1	2.85	0.45
1:G:137:GLN:CG	1:G:339:VAL:HG13	2.47	0.45
1:J:99:GLU:OE2	1:J:127:PHE:HB3	2.17	0.45
1:A:156:GLY:O	1:A:157:ASP:HB2	2.16	0.44
1:A:372:ARG:CZ	1:A:372:ARG:HA	2.47	0.44
1:I:279:TYR:O	1:I:283:MET:HG2	2.16	0.44
1:J:66:THR:O	1:J:67:LEU:HB2	2.17	0.44
1:B:43:VAL:CG1	1:B:44:MET:N	2.80	0.44
1:E:33:SER:O	1:E:70:PRO:HD2	2.18	0.44
1:E:121:GLN:HG3	1:E:125:GLU:OE1	2.18	0.44
1:G:37:ARG:HG3	1:G:38:PRO:HD2	1.97	0.44
1:J:120:THR:HG23	1:J:124:PHE:CD1	2.51	0.44
1:B:147:ARG:HE	1:B:296:ASN:ND2	2.15	0.44
1:B:270:GLU:HG2	1:B:271:SER:N	2.32	0.44
1:D:37:ARG:HG3	1:D:38:PRO:CD	2.47	0.44
1:E:57:GLU:HG2	1:E:61:LYS:HE2	1.99	0.44
1:H:181:ALA:O	1:H:184:ASP:HB2	2.18	0.44
1:C:111:ASN:HB3	1:C:116:ARG:HH12	1.82	0.44
1:C:189:LEU:HD23	1:C:209:VAL:HG13	1.99	0.44
1:E:99:GLU:HA	1:E:128:ASN:O	2.18	0.44
1:E:166:TYR:CD1	1:E:289:ILE:HD13	2.52	0.44
1:F:31:PHE:CD2	1:F:55:GLY:HA2	2.52	0.44
1:F:63:GLY:HA2	1:H:287:ILE:HD12	2.00	0.44
1:F:108:ALA:O	1:F:111:ASN:HB2	2.17	0.44
1:F:317:ILE:HG22	1:F:327:ILE:HD13	1.98	0.44
1:G:44:MET:O	1:G:44:MET:HG2	2.17	0.44
1:G:288:ASP:O	1:G:291:LYS:HD2	2.18	0.44
1:J:10:CYS:HA	1:J:18:LYS:O	2.18	0.44
1:J:166:TYR:CE2	1:J:289:ILE:HG12	2.52	0.44
1:A:304:THR:HA	1:A:309:ILE:HG21	2.00	0.44
1:B:109:PRO:HB2	1:B:161:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:GLU:HB2	1:C:134:VAL:HG22	1.98	0.44
1:D:37:ARG:HG3	1:D:38:PRO:HD2	1.99	0.44
1:D:149:THR:CB	1:D:292:ASP:HB2	2.47	0.44
1:H:289:ILE:O	1:H:293:LEU:HG	2.17	0.44
1:J:243:PRO:O	1:J:244:ASP:HB2	2.18	0.44
1:C:195:GLU:HG3	1:C:196:ARG:N	2.33	0.44
1:D:24:ASP:O	1:D:25:ASP:HB3	2.18	0.44
1:D:305:MET:HE3	1:D:336:LYS:HB2	1.99	0.44
1:H:306:TYR:HD1	1:H:306:TYR:N	2.14	0.44
1:I:111:ASN:HB3	1:I:116:ARG:HH12	1.82	0.44
1:I:260:THR:CG2	1:I:267:ILE:HG23	2.48	0.44
1:J:137:GLN:HG3	1:J:154:ASP:OD2	2.18	0.44
1:J:253:GLU:HA	1:J:256:ARG:HB3	1.99	0.44
1:C:107:GLU:CD	1:C:116:ARG:HH12	2.20	0.44
1:D:31:PHE:CD2	1:D:55:GLY:HA2	2.52	0.44
1:J:110:LEU:HD12	1:J:177:ARG:HB2	2.00	0.44
1:B:140:LEU:HB3	1:B:342:GLY:HA3	1.98	0.44
1:D:8:LEU:HB2	1:D:102:PRO:O	2.17	0.44
1:F:79:TRP:HZ2	1:F:115:ASN:ND2	2.15	0.44
1:F:135:ALA:HB1	1:F:140:LEU:HD11	1.99	0.44
1:F:156:GLY:O	1:F:157:ASP:HB3	2.18	0.44
1:H:347:ALA:HA	1:H:352:PHE:CD2	2.53	0.44
1:J:31:PHE:HE2	1:J:85:ILE:HG23	1.83	0.44
1:D:124:PHE:CG	1:D:359:LYS:HD3	2.53	0.44
1:G:219:VAL:HG22	1:G:258:PRO:HB3	1.99	0.44
1:H:43:VAL:HG23	1:J:171:LEU:CD2	2.48	0.44
1:H:188:TYR:OH	1:H:192:ILE:HD11	2.18	0.44
1:I:154:ASP:OD1	1:I:339:VAL:HG22	2.18	0.44
1:F:7:ALA:HA	1:F:102:PRO:HB2	2.00	0.43
1:F:140:LEU:HD23	1:F:343:GLY:CA	2.48	0.43
1:F:171:LEU:CD1	1:F:171:LEU:H	2.31	0.43
1:F:208:ILE:HG21	1:F:242:LEU:HD11	2.00	0.43
1:G:36:GLY:HA3	1:G:53:TYR:HB2	2.00	0.43
1:G:70:PRO:O	1:G:76:ILE:HG23	2.18	0.43
1:H:6:THR:HG23	1:H:7:ALA:N	2.33	0.43
1:I:9:VAL:HG21	1:I:344:SER:HA	1.99	0.43
1:C:35:VAL:HA	1:C:53:TYR:O	2.18	0.43
1:E:36:GLY:HA3	1:E:65:LEU:HG	1.99	0.43
1:G:84:LYS:O	1:G:87:HIS:HB3	2.17	0.43
1:H:272:ALA:HB3	1:H:276:GLU:HB2	1.99	0.43
1:J:16:LEU:HD23	1:J:32:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:O	1:A:94:LEU:HB2	2.17	0.43
1:B:109:PRO:HB2	1:B:161:HIS:ND1	2.33	0.43
1:C:99:GLU:O	1:C:130:PRO:HD3	2.17	0.43
1:D:12:ASN:H	1:D:106:THR:HG22	1.82	0.43
1:D:99:GLU:O	1:D:130:PRO:HD3	2.19	0.43
1:G:36:GLY:HA3	1:G:65:LEU:HG	2.00	0.43
1:I:10:CYS:HA	1:I:18:LYS:O	2.18	0.43
1:I:257:CYS:CB	1:I:258:PRO:HD3	2.48	0.43
1:J:294:TYR:HB3	1:J:327:ILE:CD1	2.49	0.43
1:A:288:ASP:O	1:A:289:ILE:HG13	2.18	0.43
1:C:181:ALA:O	1:C:184:ASP:HB2	2.17	0.43
1:I:124:PHE:O	1:I:128:ASN:HA	2.18	0.43
1:J:124:PHE:CZ	1:J:132:MET:HG2	2.54	0.43
1:J:158:GLY:HA2	1:J:183:ARG:HD3	1.99	0.43
1:F:43:VAL:HG13	1:F:44:MET:H	1.83	0.43
1:G:264:PRO:HG2	1:G:272:ALA:C	2.38	0.43
1:H:43:VAL:HG23	1:J:171:LEU:HD21	2.00	0.43
1:H:283:MET:HA	1:H:290:ARG:HH21	1.82	0.43
1:I:286:ASP:CB	1:I:289:ILE:HD12	2.41	0.43
1:J:62:ARG:HE	1:J:207:GLU:HB3	1.83	0.43
1:J:109:PRO:HB2	1:J:161:HIS:CD2	2.53	0.43
1:J:171:LEU:C	1:J:171:LEU:HD12	2.38	0.43
1:A:7:ALA:HA	1:A:102:PRO:HB2	1.99	0.43
1:A:29:ALA:HB2	1:A:93:GLU:HB2	2.01	0.43
1:A:133:TYR:HB2	1:A:356:TRP:HB2	1.99	0.43
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.53	0.43
1:B:71:ILE:HG12	1:B:76:ILE:CG1	2.45	0.43
1:B:111:ASN:HB3	1:B:116:ARG:HH12	1.84	0.43
1:C:137:GLN:HG3	1:C:339:VAL:CG1	2.42	0.43
1:E:289:ILE:O	1:E:293:LEU:HG	2.18	0.43
1:E:304:THR:O	1:E:309:ILE:HG21	2.19	0.43
1:J:11:ASP:OD2	1:J:106:THR:HG21	2.19	0.43
1:J:118:LYS:NZ	1:J:122:ILE:HD11	2.33	0.43
1:J:264:PRO:HG2	1:J:271:SER:O	2.19	0.43
1:A:137:GLN:HG3	1:A:339:VAL:HG13	2.01	0.43
1:D:50:LYS:HB3	1:D:52:SER:O	2.18	0.43
1:D:124:PHE:CD2	1:D:359:LYS:HB2	2.53	0.43
1:D:286:ASP:CB	1:D:289:ILE:HD12	2.48	0.43
1:F:90:PHE:O	1:F:94:LEU:HB2	2.19	0.43
1:F:272:ALA:HB3	1:F:276:GLU:HB2	2.01	0.43
1:I:163:VAL:HA	1:I:175:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:LYS:HA	1:I:217:CYS:SG	2.59	0.43
1:J:124:PHE:HD2	1:J:359:LYS:CD	2.31	0.43
1:J:299:MET:HB3	1:J:304:THR:CG2	2.49	0.43
1:B:137:GLN:HG2	1:B:154:ASP:OD2	2.18	0.43
1:F:6:THR:CG2	1:F:22:ALA:HB3	2.48	0.43
1:G:6:THR:O	1:G:7:ALA:HB3	2.18	0.43
1:G:338:SER:HA	1:G:341:ILE:CG2	2.47	0.43
1:I:111:ASN:HB3	1:I:116:ARG:NH1	2.33	0.43
1:J:70:PRO:HB2	1:J:82:MET:SD	2.59	0.43
1:J:248:ILE:HG22	1:J:250:ILE:HG23	2.01	0.43
1:C:16:LEU:N	1:C:16:LEU:HD23	2.34	0.43
1:C:205:GLU:H	1:C:205:GLU:HG2	1.65	0.43
1:C:289:ILE:HG22	1:C:293:LEU:CD1	2.49	0.43
1:E:21:PHE:HZ	1:E:96:VAL:HG11	1.82	0.43
1:E:124:PHE:CD2	1:E:359:LYS:HB2	2.54	0.43
1:G:365:ALA:HB3	1:G:369:ILE:HD13	2.01	0.43
1:H:9:VAL:O	1:H:19:ALA:HA	2.18	0.43
1:H:32:PRO:HG3	1:H:59:GLN:HB2	2.01	0.43
1:H:116:ARG:CG	1:H:116:ARG:NH1	2.72	0.43
1:I:284:LYS:HB2	1:I:284:LYS:NZ	2.34	0.43
1:A:61:LYS:O	1:A:63:GLY:N	2.50	0.43
1:B:196:ARG:NH1	1:B:196:ARG:HB3	2.34	0.43
1:D:140:LEU:HG	1:D:346:LEU:HD12	2.01	0.43
1:D:230:ALA:HA	1:D:236:LEU:CD2	2.48	0.43
1:E:109:PRO:HD3	1:E:137:GLN:NE2	2.34	0.43
1:E:256:ARG:O	1:E:259:GLU:HB3	2.19	0.43
1:H:24:ASP:HB3	1:H:28:ARG:HH12	1.83	0.43
1:H:70:PRO:O	1:H:76:ILE:HG12	2.19	0.43
1:J:290:ARG:HB3	1:J:294:TYR:CE2	2.54	0.43
1:A:279:TYR:OH	1:A:317:ILE:HA	2.19	0.42
1:F:35:VAL:HG11	1:F:81:ASP:HB2	1.99	0.42
1:G:189:LEU:HD23	1:G:209:VAL:HG13	1.99	0.42
1:H:63:GLY:HA3	1:J:288:ASP:OD2	2.19	0.42
1:J:291:LYS:HA	1:J:325:MET:HG3	2.01	0.42
1:C:294:TYR:HA	1:C:297:ASN:OD1	2.19	0.42
1:D:94:LEU:HB3	1:D:96:VAL:HG22	2.01	0.42
1:E:172:PRO:HA	1:E:175:ILE:HG12	2.01	0.42
1:E:252:ASN:HA	1:E:255:PHE:CE2	2.55	0.42
1:F:101:HIS:HA	1:F:102:PRO:HD3	1.88	0.42
1:F:149:THR:HG21	1:F:292:ASP:OD2	2.19	0.42
1:G:111:ASN:HB3	1:G:116:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:LEU:HB3	1:G:352:PHE:CD1	2.54	0.42
1:H:142:LEU:HD22	1:H:165:ILE:HG12	2.01	0.42
1:J:221:LEU:HA	1:J:312:ARG:HG2	2.01	0.42
1:D:53:TYR:CB	1:D:65:LEU:HD21	2.47	0.42
1:E:294:TYR:HB3	1:E:327:ILE:HD13	2.01	0.42
1:F:6:THR:HG22	1:F:22:ALA:CB	2.47	0.42
1:G:150:GLY:CA	1:G:296:ASN:HB2	2.49	0.42
1:G:200:PHE:HA	1:G:205:GLU:OE2	2.19	0.42
1:H:164:PRO:HG3	1:H:174:ALA:CB	2.47	0.42
1:A:195:GLU:HG3	1:A:196:ARG:N	2.34	0.42
1:B:54:VAL:HG21	1:B:85:ILE:HA	2.02	0.42
1:D:71:ILE:HG12	1:D:76:ILE:CG1	2.48	0.42
1:I:218:TYR:HA	1:I:307:PRO:HD2	2.01	0.42
1:A:33:SER:O	1:A:70:PRO:HD2	2.20	0.42
1:A:264:PRO:O	1:A:267:ILE:HG12	2.19	0.42
1:F:47:MET:HG2	1:F:50:LYS:O	2.20	0.42
1:G:7:ALA:CB	1:G:102:PRO:HB2	2.49	0.42
1:I:21:PHE:HB2	1:I:24:ASP:OD2	2.20	0.42
1:I:260:THR:HG21	1:I:267:ILE:HG23	2.02	0.42
1:A:166:TYR:CG	1:A:167:GLU:N	2.87	0.42
1:C:314:GLN:OE1	1:C:328:LYS:HA	2.19	0.42
1:E:10:CYS:HA	1:E:18:LYS:O	2.19	0.42
1:E:124:PHE:CE2	1:E:359:LYS:HB2	2.53	0.42
1:F:90:PHE:CB	1:F:98:PRO:HG3	2.50	0.42
1:G:177:ARG:HB3	1:G:177:ARG:HH11	1.84	0.42
1:G:282:ILE:HG22	1:G:290:ARG:HG2	2.02	0.42
1:I:299:MET:HB3	1:I:304:THR:CG2	2.49	0.42
1:J:200:PHE:CB	1:J:205:GLU:HG3	2.50	0.42
1:J:223:PHE:HB2	1:J:259:GLU:CD	2.40	0.42
1:B:133:TYR:CD1	1:B:356:TRP:HA	2.54	0.42
1:E:61:LYS:HG2	1:G:291:LYS:CE	2.50	0.42
1:E:314:GLN:HG3	1:E:329:ILE:HG12	2.01	0.42
1:J:282:ILE:HG21	1:J:290:ARG:HG2	2.00	0.42
1:B:21:PHE:HE1	1:B:96:VAL:HG21	1.84	0.42
1:B:136:ILE:HG21	1:B:375:PHE:CZ	2.55	0.42
1:D:142:LEU:HD22	1:D:165:ILE:HG21	2.02	0.42
1:D:289:ILE:HG22	1:D:293:LEU:CD1	2.49	0.42
1:G:300:SER:HA	1:G:335:ARG:HB2	2.01	0.42
1:A:331:ALA:HB1	1:A:335:ARG:HH11	1.85	0.42
1:C:151:ILE:CD1	1:C:164:PRO:HA	2.50	0.42
1:D:8:LEU:HD21	1:D:90:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:CD2	1:D:261:LEU:HA	2.50	0.42
1:D:255:PHE:C	1:D:258:PRO:HD2	2.40	0.42
1:E:1:ASP:C	1:E:2:GLU:HG2	2.39	0.42
1:G:142:LEU:HD22	1:G:165:ILE:CG1	2.48	0.42
1:I:105:LEU:O	1:I:134:VAL:HA	2.20	0.42
1:I:258:PRO:HG3	1:I:306:TYR:CD2	2.54	0.42
1:I:313:MET:HB2	1:I:329:ILE:HG13	2.01	0.42
1:J:99:GLU:O	1:J:130:PRO:HD3	2.20	0.42
1:B:304:THR:HB	1:B:309:ILE:HG21	2.00	0.42
1:C:253:GLU:HA	1:C:256:ARG:HB3	2.02	0.42
1:D:133:TYR:HD1	1:D:357:ILE:H	1.66	0.42
1:D:195:GLU:HG3	1:D:196:ARG:N	2.35	0.42
1:E:47:MET:HA	1:G:166:TYR:HE2	1.82	0.42
1:H:220:ALA:O	1:H:312:ARG:HD2	2.19	0.42
1:D:136:ILE:HD13	1:D:375:PHE:CE2	2.55	0.41
1:D:166:TYR:HD1	1:D:166:TYR:HA	1.74	0.41
1:E:208:ILE:HG21	1:E:242:LEU:CD1	2.47	0.41
1:A:12:ASN:H	1:A:106:THR:HG22	1.85	0.41
1:A:283:MET:HA	1:A:290:ARG:HH21	1.84	0.41
1:A:346:LEU:HB2	1:A:352:PHE:CD1	2.55	0.41
1:A:353:GLN:HG3	1:A:356:TRP:CZ2	2.55	0.41
1:C:151:ILE:HG12	1:C:293:LEU:CD2	2.45	0.41
1:D:35:VAL:HG22	1:D:54:VAL:HG23	2.01	0.41
1:D:172:PRO:HA	1:D:175:ILE:HG12	2.02	0.41
1:D:305:MET:CE	1:D:336:LYS:HD2	2.50	0.41
1:F:105:LEU:O	1:F:134:VAL:HA	2.20	0.41
1:H:166:TYR:CD2	1:H:289:ILE:HD11	2.54	0.41
1:H:260:THR:HG23	1:H:267:ILE:HG23	2.02	0.41
1:H:260:THR:HG23	1:H:267:ILE:CG2	2.51	0.41
1:I:118:LYS:NZ	1:I:122:ILE:HD11	2.35	0.41
1:I:188:TYR:CD1	1:I:267:ILE:HG22	2.56	0.41
1:I:314:GLN:OE1	1:I:328:LYS:HA	2.20	0.41
1:A:300:SER:HA	1:A:335:ARG:HB2	2.02	0.41
1:B:43:VAL:HG12	1:B:44:MET:N	2.35	0.41
1:C:272:ALA:HB3	1:C:276:GLU:CB	2.49	0.41
1:C:358:THR:HG22	1:C:359:LYS:N	2.35	0.41
1:D:54:VAL:HG21	1:D:85:ILE:HA	2.01	0.41
1:D:196:ARG:HD2	1:D:198:TYR:CE2	2.56	0.41
1:F:104:LEU:CD2	1:F:347:ALA:HB2	2.49	0.41
1:H:123:MET:O	1:H:127:PHE:O	2.38	0.41
1:F:171:LEU:HD12	1:F:171:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:MET:HG2	1:G:290:ARG:NH2	2.35	0.41
1:H:37:ARG:O	1:H:66:THR:HG23	2.21	0.41
1:I:276:GLU:HA	1:I:279:TYR:CD1	2.56	0.41
1:J:140:LEU:HB3	1:J:342:GLY:HA3	2.03	0.41
1:J:275:HIS:CD2	1:J:316:GLU:HB3	2.56	0.41
1:A:27:PRO:HD3	1:A:340:TRP:CH2	2.56	0.41
1:C:294:TYR:HB3	1:C:327:ILE:HD13	2.03	0.41
1:E:35:VAL:HG11	1:E:81:ASP:HB2	2.01	0.41
1:E:299:MET:HB3	1:E:304:THR:CG2	2.47	0.41
1:I:7:ALA:C	1:I:8:LEU:HD22	2.41	0.41
1:I:124:PHE:CE2	1:I:359:LYS:HD3	2.55	0.41
1:J:18:LYS:HA	1:J:30:VAL:HG12	2.02	0.41
1:J:79:TRP:O	1:J:82:MET:HB2	2.21	0.41
1:J:192:ILE:O	1:J:195:GLU:HG3	2.20	0.41
1:A:46:GLY:HA3	1:C:166:TYR:HB3	2.02	0.41
1:B:42:GLY:O	1:B:43:VAL:CB	2.69	0.41
1:C:46:GLY:HA3	1:E:166:TYR:CD2	2.55	0.41
1:C:250:ILE:HD12	1:C:254:ARG:CG	2.45	0.41
1:E:284:LYS:HB2	1:E:284:LYS:HZ2	1.85	0.41
1:F:272:ALA:HB3	1:F:276:GLU:CB	2.51	0.41
1:H:79:TRP:HZ2	1:H:115:ASN:HD22	1.68	0.41
1:H:90:PHE:HA	1:H:94:LEU:HD12	2.02	0.41
1:I:151:ILE:HB	1:I:293:LEU:CD2	2.35	0.41
1:I:281:SER:O	1:I:285:CYS:SG	2.78	0.41
1:I:305:MET:SD	1:I:335:ARG:HG2	2.61	0.41
1:J:70:PRO:O	1:J:76:ILE:HA	2.20	0.41
1:C:104:LEU:HD23	1:C:347:ALA:HB2	2.03	0.41
1:D:70:PRO:HG3	1:D:85:ILE:HD11	2.03	0.41
1:G:105:LEU:O	1:G:134:VAL:HA	2.21	0.41
1:J:188:TYR:CE1	1:J:267:ILE:HG22	2.55	0.41
1:A:317:ILE:HD12	1:A:329:ILE:HD11	2.02	0.41
1:D:278:THR:HG22	1:D:282:ILE:CD1	2.51	0.41
1:E:61:LYS:HG2	1:G:291:LYS:NZ	2.36	0.41
1:G:12:ASN:HB2	1:G:71:ILE:HD11	2.02	0.41
1:H:31:PHE:HB2	1:H:55:GLY:HA2	2.03	0.41
1:I:197:GLY:HA2	1:J:113:LYS:HG3	2.02	0.41
1:J:105:LEU:O	1:J:134:VAL:HA	2.20	0.41
1:J:151:ILE:HD12	1:J:164:PRO:HA	2.02	0.41
1:J:250:ILE:HD12	1:J:254:ARG:CG	2.47	0.41
1:A:35:VAL:HG11	1:A:81:ASP:HB2	2.03	0.41
1:B:142:LEU:HG	1:B:147:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:THR:O	1:B:296:ASN:HB2	2.20	0.41
1:C:108:ALA:O	1:C:111:ASN:HB2	2.21	0.41
1:C:122:ILE:O	1:C:126:THR:HB	2.20	0.41
1:C:140:LEU:O	1:C:342:GLY:HA3	2.20	0.41
1:C:255:PHE:C	1:C:258:PRO:HD2	2.41	0.41
1:F:164:PRO:HD2	1:F:175:ILE:HG22	2.03	0.41
1:F:253:GLU:HA	1:F:256:ARG:HB3	2.03	0.41
1:G:70:PRO:O	1:G:76:ILE:HG12	2.21	0.41
1:G:220:ALA:HB1	1:G:226:GLU:OE2	2.21	0.41
1:H:211:ASP:O	1:H:215:LYS:HG2	2.20	0.41
1:H:278:THR:HG22	1:H:282:ILE:CD1	2.51	0.41
1:I:104:LEU:HD12	1:I:133:TYR:O	2.20	0.41
1:I:133:TYR:CE1	1:I:357:ILE:HG12	2.56	0.41
1:A:241:GLU:OE1	1:A:247:VAL:HG12	2.21	0.41
1:B:124:PHE:CE2	1:B:359:LYS:HB2	2.56	0.41
1:B:242:LEU:HD23	1:B:242:LEU:C	2.41	0.41
1:D:35:VAL:HA	1:D:53:TYR:O	2.21	0.41
1:E:278:THR:O	1:E:282:ILE:HG13	2.20	0.41
1:F:8:LEU:HA	1:F:20:GLY:O	2.21	0.41
1:F:17:VAL:CG2	1:F:33:SER:HB3	2.51	0.41
1:G:124:PHE:CE2	1:G:359:LYS:HB2	2.56	0.41
1:I:31:PHE:CE2	1:I:85:ILE:HG23	2.55	0.41
1:J:340:TRP:HE3	1:J:341:ILE:HD13	1.86	0.41
1:B:164:PRO:HG3	1:B:174:ALA:HB1	2.03	0.40
1:D:286:ASP:HB3	1:D:289:ILE:CG1	2.50	0.40
1:E:281:SER:HA	1:E:284:LYS:HZ2	1.85	0.40
1:H:325:MET:SD	1:H:325:MET:N	2.95	0.40
1:A:116:ARG:CB	1:A:370:VAL:HG21	2.51	0.40
1:B:21:PHE:CE1	1:B:96:VAL:HG21	2.56	0.40
1:D:47:MET:C	1:D:49:GLN:H	2.25	0.40
1:D:110:LEU:HD22	1:D:110:LEU:HA	1.79	0.40
1:F:4:GLU:HB3	1:F:5:THR:H	1.72	0.40
1:G:62:ARG:HG2	1:G:63:GLY:N	2.36	0.40
1:I:226:GLU:O	1:I:229:THR:HB	2.20	0.40
1:J:289:ILE:HG22	1:J:293:LEU:CD2	2.46	0.40
1:B:203:THR:HA	1:B:206:ARG:HB2	2.03	0.40
1:E:345:ILE:HG22	1:E:349:LEU:CD1	2.51	0.40
1:F:219:VAL:HG22	1:F:258:PRO:CB	2.51	0.40
1:H:291:LYS:HG3	1:H:292:ASP:N	2.36	0.40
1:I:175:ILE:O	1:I:175:ILE:HG13	2.20	0.40
1:I:192:ILE:CG2	1:I:256:ARG:HD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:LEU:HB3	1:I:198:TYR:HB2	2.03	0.40
1:J:70:PRO:HB3	1:J:81:ASP:OD2	2.21	0.40
1:J:287:ILE:HA	1:J:290:ARG:HH12	1.80	0.40
1:B:264:PRO:O	1:B:267:ILE:HG12	2.21	0.40
1:C:149:THR:HG22	1:C:296:ASN:ND2	2.33	0.40
1:C:289:ILE:HG22	1:C:293:LEU:HD11	2.04	0.40
1:D:63:GLY:HA3	1:F:287:ILE:CG2	2.51	0.40
1:D:260:THR:HG21	1:D:267:ILE:HG21	2.04	0.40
1:I:151:ILE:CB	1:I:293:LEU:HD22	2.36	0.40
1:I:294:TYR:HB3	1:I:327:ILE:HD13	2.04	0.40
1:J:18:LYS:HE3	1:J:337:TYR:CD1	2.56	0.40
1:J:149:THR:CG2	1:J:292:ASP:HB2	2.51	0.40
1:A:46:GLY:HA3	1:C:166:TYR:HD2	1.87	0.40
1:A:220:ALA:HB2	1:A:255:PHE:HB2	2.03	0.40
1:D:24:ASP:O	1:D:25:ASP:CB	2.69	0.40
1:E:11:ASP:OD2	1:E:106:THR:HG21	2.21	0.40
1:E:300:SER:HA	1:E:335:ARG:HB2	2.04	0.40
1:F:171:LEU:CD1	1:F:171:LEU:N	2.85	0.40
1:F:325:MET:N	1:F:325:MET:SD	2.95	0.40
1:G:177:ARG:HB3	1:G:177:ARG:NH1	2.37	0.40
1:H:121:GLN:HG3	1:H:125:GLU:OE1	2.21	0.40
1:I:140:LEU:HD23	1:I:343:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	6 33
1	B	373/377 (99%)	349 (94%)	11 (3%)	13 (4%)	3 25
1	C	373/377 (99%)	350 (94%)	14 (4%)	9 (2%)	6 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/377 (99%)	340 (91%)	17 (5%)	16 (4%)	2	22
1	E	373/377 (99%)	339 (91%)	18 (5%)	16 (4%)	2	22
1	F	373/377 (99%)	343 (92%)	17 (5%)	13 (4%)	3	25
1	G	373/377 (99%)	343 (92%)	19 (5%)	11 (3%)	4	29
1	H	373/377 (99%)	347 (93%)	15 (4%)	11 (3%)	4	29
1	I	373/377 (99%)	348 (93%)	18 (5%)	7 (2%)	8	38
1	J	373/377 (99%)	344 (92%)	21 (6%)	8 (2%)	7	36
All	All	3730/3770 (99%)	3453 (93%)	164 (4%)	113 (3%)	7	28

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ARG
1	B	6	THR
1	B	7	ALA
1	B	41	GLN
1	B	43	VAL
1	B	62	ARG
1	B	157	ASP
1	B	173	HIS
1	B	244	ASP
1	B	307	PRO
1	C	6	THR
1	C	157	ASP
1	D	14	SER
1	D	41	GLN
1	D	159	VAL
1	D	173	HIS
1	D	204	ALA
1	D	234	SER
1	E	6	THR
1	E	49	GLN
1	F	4	GLU
1	F	6	THR
1	F	45	VAL
1	F	286	ASP
1	G	6	THR
1	G	48	GLY
1	G	173	HIS
1	H	6	THR

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Mol	Chain	Res	Type
1	H	43	VAL
1	H	234	SER
1	H	244	ASP
1	I	286	ASP
1	J	173	HIS
1	J	234	SER
1	J	285	CYS
1	A	43	VAL
1	A	157	ASP
1	A	173	HIS
1	A	222	ASP
1	B	234	SER
1	C	43	VAL
1	C	244	ASP
1	D	25	ASP
1	D	244	ASP
1	D	352	PHE
1	E	3	ASP
1	E	7	ALA
1	E	43	VAL
1	E	57	GLU
1	E	157	ASP
1	E	173	HIS
1	E	244	ASP
1	E	286	ASP
1	E	363	ASP
1	F	7	ALA
1	F	41	GLN
1	F	43	VAL
1	F	44	MET
1	F	167	GLU
1	F	173	HIS
1	G	25	ASP
1	G	45	VAL
1	G	244	ASP
1	H	173	HIS
1	I	173	HIS
1	J	6	THR
1	J	244	ASP
1	A	342	GLY
1	B	273	GLY
1	B	308	GLY

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Mol	Chain	Res	Type
1	C	41	GLN
1	C	273	GLY
1	C	286	ASP
1	D	2	GLU
1	D	286	ASP
1	E	41	GLN
1	E	45	VAL
1	E	234	SER
1	E	273	GLY
1	F	273	GLY
1	G	41	GLN
1	G	43	VAL
1	G	286	ASP
1	H	45	VAL
1	H	166	TYR
1	I	7	ALA
1	I	197	GLY
1	I	230	ALA
1	A	347	ALA
1	D	6	THR
1	D	43	VAL
1	D	245	GLY
1	F	157	ASP
1	G	42	GLY
1	G	63	GLY
1	H	195	GLU
1	H	350	SER
1	J	197	GLY
1	A	7	ALA
1	C	352	PHE
1	D	49	GLN
1	H	245	GLY
1	J	157	ASP
1	A	289	ILE
1	C	245	GLY
1	J	245	GLY
1	I	48	GLY
1	I	273	GLY
1	B	245	GLY
1	E	15	GLY
1	F	46	GLY
1	D	158	GLY

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Mol	Chain	Res	Type
1	H	345	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/320 (99%)	302 (95%)	16 (5%)	24	49
1	B	318/320 (99%)	301 (95%)	17 (5%)	22	47
1	C	318/320 (99%)	297 (93%)	21 (7%)	16	41
1	D	318/320 (99%)	296 (93%)	22 (7%)	15	40
1	E	318/320 (99%)	301 (95%)	17 (5%)	22	47
1	F	318/320 (99%)	295 (93%)	23 (7%)	14	39
1	G	318/320 (99%)	300 (94%)	18 (6%)	20	45
1	H	318/320 (99%)	298 (94%)	20 (6%)	18	43
1	I	318/320 (99%)	299 (94%)	19 (6%)	19	44
1	J	318/320 (99%)	302 (95%)	16 (5%)	24	49
All	All	3180/3200 (99%)	2991 (94%)	189 (6%)	23	45

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	37	ARG
1	A	40	HIS
1	A	49	GLN
1	A	61	LYS
1	A	69	TYR
1	A	195	GLU
1	A	196	ARG
1	A	202	THR
1	A	235	SER
1	A	291	LYS
1	A	309	ILE

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	346	LEU
1	A	356	TRP
1	A	372	ARG
1	B	8	LEU
1	B	33	SER
1	B	39	ARG
1	B	40	HIS
1	B	69	TYR
1	B	87	HIS
1	B	140	LEU
1	B	149	THR
1	B	155	SER
1	B	202	THR
1	B	205	GLU
1	B	227	MET
1	B	253	GLU
1	B	303	THR
1	B	320	LEU
1	B	335	ARG
1	B	356	TRP
1	C	3	ASP
1	C	6	THR
1	C	16	LEU
1	C	33	SER
1	C	69	TYR
1	C	87	HIS
1	C	107	GLU
1	C	123	MET
1	C	151	ILE
1	C	157	ASP
1	C	166	TYR
1	C	196	ARG
1	C	205	GLU
1	C	244	ASP
1	C	246	GLN
1	C	270	GLU
1	C	325	MET
1	C	335	ARG
1	C	352	PHE
1	C	356	TRP
1	C	372	ARG

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Mol	Chain	Res	Type
1	D	6	THR
1	D	12	ASN
1	D	28	ARG
1	D	37	ARG
1	D	69	TYR
1	D	87	HIS
1	D	110	LEU
1	D	159	VAL
1	D	162	ASN
1	D	166	TYR
1	D	179	ASP
1	D	195	GLU
1	D	196	ARG
1	D	203	THR
1	D	257	CYS
1	D	270	GLU
1	D	291	LYS
1	D	314	GLN
1	D	324	THR
1	D	356	TRP
1	D	358	THR
1	D	375	PHE
1	E	2	GLU
1	E	45	VAL
1	E	49	GLN
1	E	59	GLN
1	E	69	TYR
1	E	140	LEU
1	E	149	THR
1	E	166	TYR
1	E	225	ASN
1	E	227	MET
1	E	257	CYS
1	E	289	ILE
1	E	291	LYS
1	E	358	THR
1	E	359	LYS
1	E	364	GLU
1	E	372	ARG
1	F	5	THR
1	F	6	THR
1	F	33	SER

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Mol	Chain	Res	Type
1	F	37	ARG
1	F	44	MET
1	F	45	VAL
1	F	47	MET
1	F	69	TYR
1	F	87	HIS
1	F	113	LYS
1	F	123	MET
1	F	166	TYR
1	F	171	LEU
1	F	179	ASP
1	F	183	ARG
1	F	195	GLU
1	F	196	ARG
1	F	289	ILE
1	F	306	TYR
1	F	335	ARG
1	F	356	TRP
1	F	360	GLN
1	F	372	ARG
1	G	12	ASN
1	G	37	ARG
1	G	44	MET
1	G	69	TYR
1	G	106	THR
1	G	110	LEU
1	G	140	LEU
1	G	166	TYR
1	G	177	ARG
1	G	183	ARG
1	G	195	GLU
1	G	196	ARG
1	G	244	ASP
1	G	263	GLN
1	G	270	GLU
1	G	291	LYS
1	G	327	ILE
1	G	358	THR
1	H	8	LEU
1	H	33	SER
1	H	37	ARG
1	H	39	ARG

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Mol	Chain	Res	Type
1	H	45	VAL
1	H	69	TYR
1	H	87	HIS
1	H	106	THR
1	H	116	ARG
1	H	117	GLU
1	H	166	TYR
1	H	195	GLU
1	H	283	MET
1	H	291	LYS
1	H	306	TYR
1	H	346	LEU
1	H	349	LEU
1	H	355	MET
1	H	356	TRP
1	H	358	THR
1	I	6	THR
1	I	33	SER
1	I	39	ARG
1	I	47	MET
1	I	69	TYR
1	I	87	HIS
1	I	113	LYS
1	I	123	MET
1	I	137	GLN
1	I	166	TYR
1	I	183	ARG
1	I	196	ARG
1	I	224	GLU
1	I	257	CYS
1	I	292	ASP
1	I	315	LYS
1	I	334	GLU
1	I	356	TRP
1	I	358	THR
1	J	6	THR
1	J	39	ARG
1	J	47	MET
1	J	69	TYR
1	J	87	HIS
1	J	123	MET
1	J	140	LEU

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Mol	Chain	Res	Type
1	J	153	LEU
1	J	195	GLU
1	J	196	ARG
1	J	270	GLU
1	J	292	ASP
1	J	293	LEU
1	J	334	GLU
1	J	335	ARG
1	J	356	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	49	GLN
1	A	137	GLN
1	A	162	ASN
1	A	246	GLN
1	A	297	ASN
1	A	353	GLN
1	A	360	GLN
1	B	73	HIS
1	B	88	HIS
1	B	92	ASN
1	B	263	GLN
1	B	296	ASN
1	B	297	ASN
1	B	314	GLN
1	B	353	GLN
1	B	360	GLN
1	C	88	HIS
1	C	92	ASN
1	C	137	GLN
1	C	296	ASN
1	C	360	GLN
1	D	73	HIS
1	D	88	HIS
1	D	92	ASN
1	D	225	ASN
1	D	296	ASN
1	D	297	ASN
1	E	12	ASN

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Mol	Chain	Res	Type
1	E	40	HIS
1	E	49	GLN
1	E	88	HIS
1	E	92	ASN
1	E	137	GLN
1	E	225	ASN
1	E	296	ASN
1	E	297	ASN
1	E	314	GLN
1	E	353	GLN
1	F	40	HIS
1	F	73	HIS
1	F	88	HIS
1	F	92	ASN
1	F	296	ASN
1	F	297	ASN
1	F	353	GLN
1	G	12	ASN
1	G	41	GLN
1	G	73	HIS
1	G	88	HIS
1	G	92	ASN
1	G	246	GLN
1	G	296	ASN
1	G	297	ASN
1	H	161	HIS
1	H	246	GLN
1	H	297	ASN
1	H	314	GLN
1	H	353	GLN
1	I	121	GLN
1	I	137	GLN
1	I	297	ASN
1	I	353	GLN
1	I	354	GLN
1	J	88	HIS
1	J	92	ASN
1	J	162	ASN
1	J	246	GLN
1	J	296	ASN
1	J	297	ASN
1	J	353	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

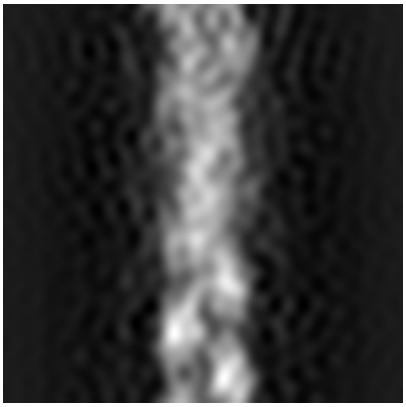
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6181. These allow visual inspection of the internal detail of the map and identification of artifacts.

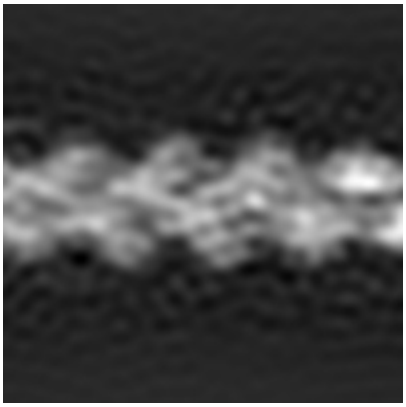
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



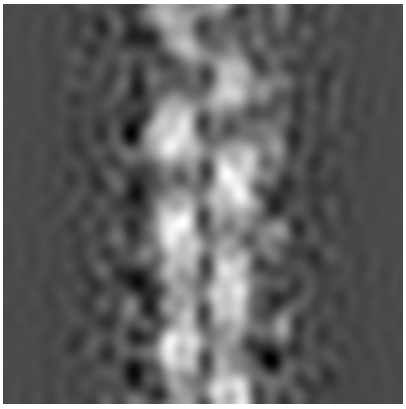
Y

Z

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

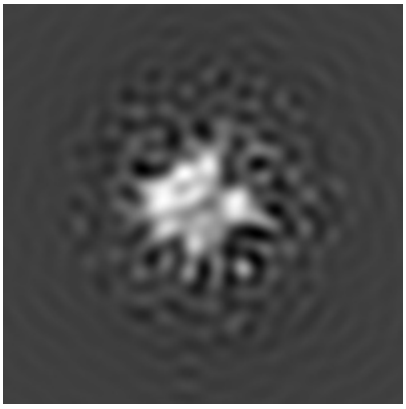
6.2 Central slices

6.2.1 Primary map



X Index: 50

Y Index: 50

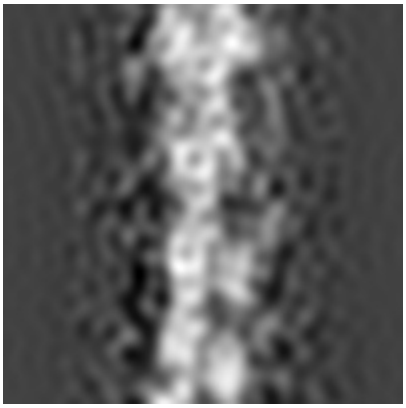


Z Index: 50

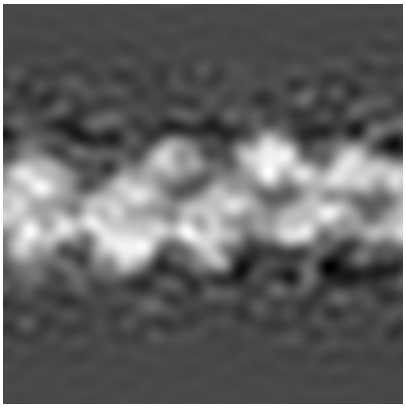
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

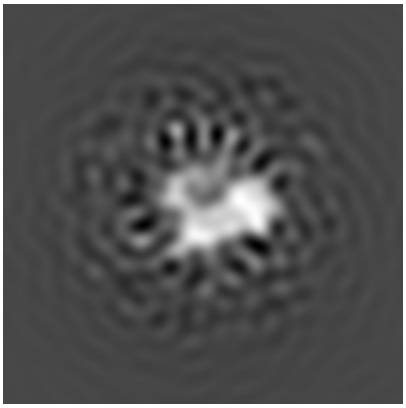
6.3.1 Primary map



X Index: 56



Y Index: 54

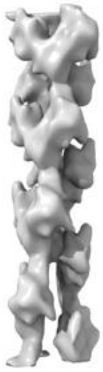


Z Index: 41

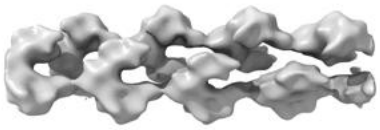
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

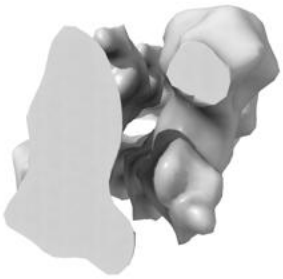
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

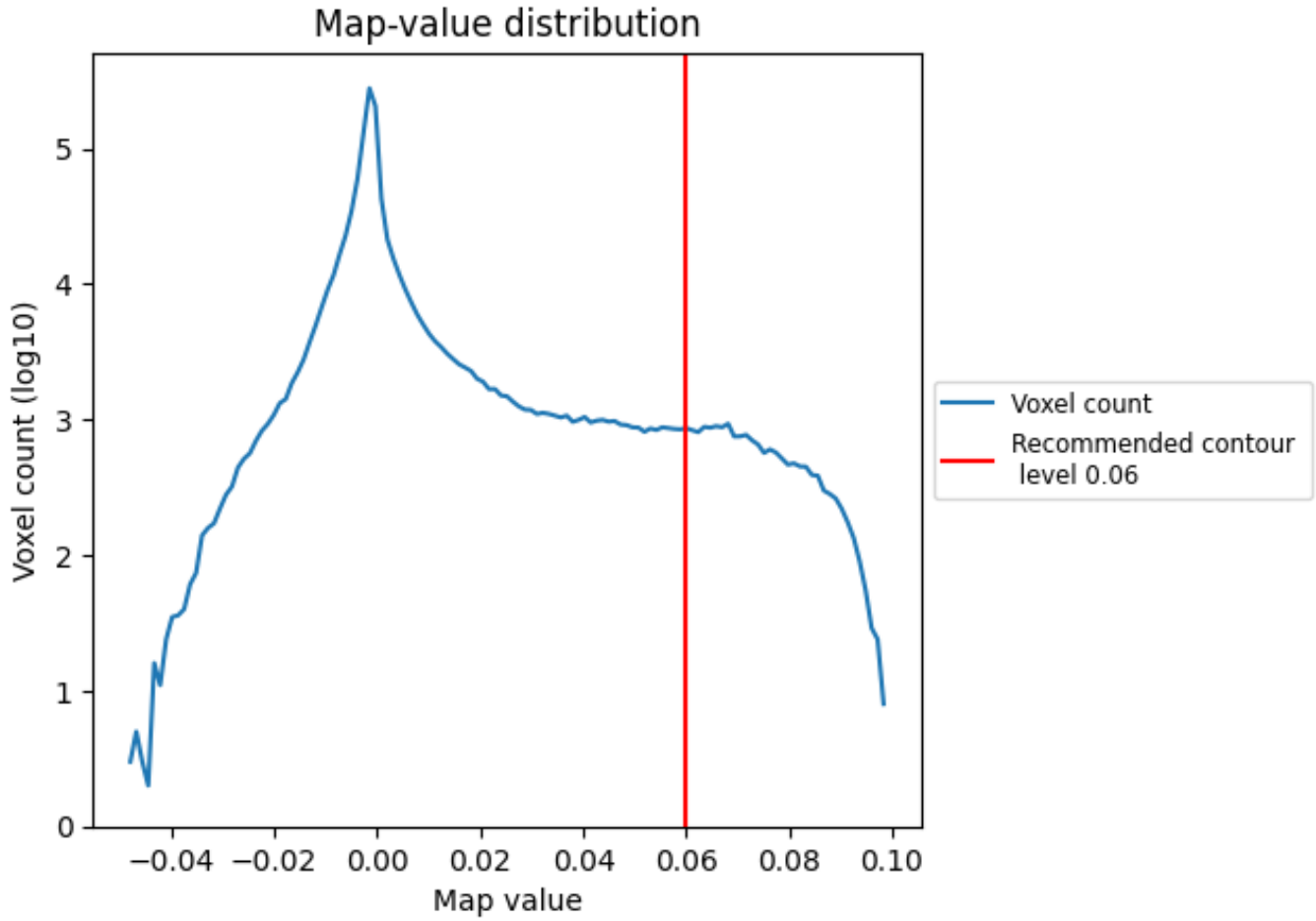
6.5 Mask visualisation (i)

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

7 Map analysis

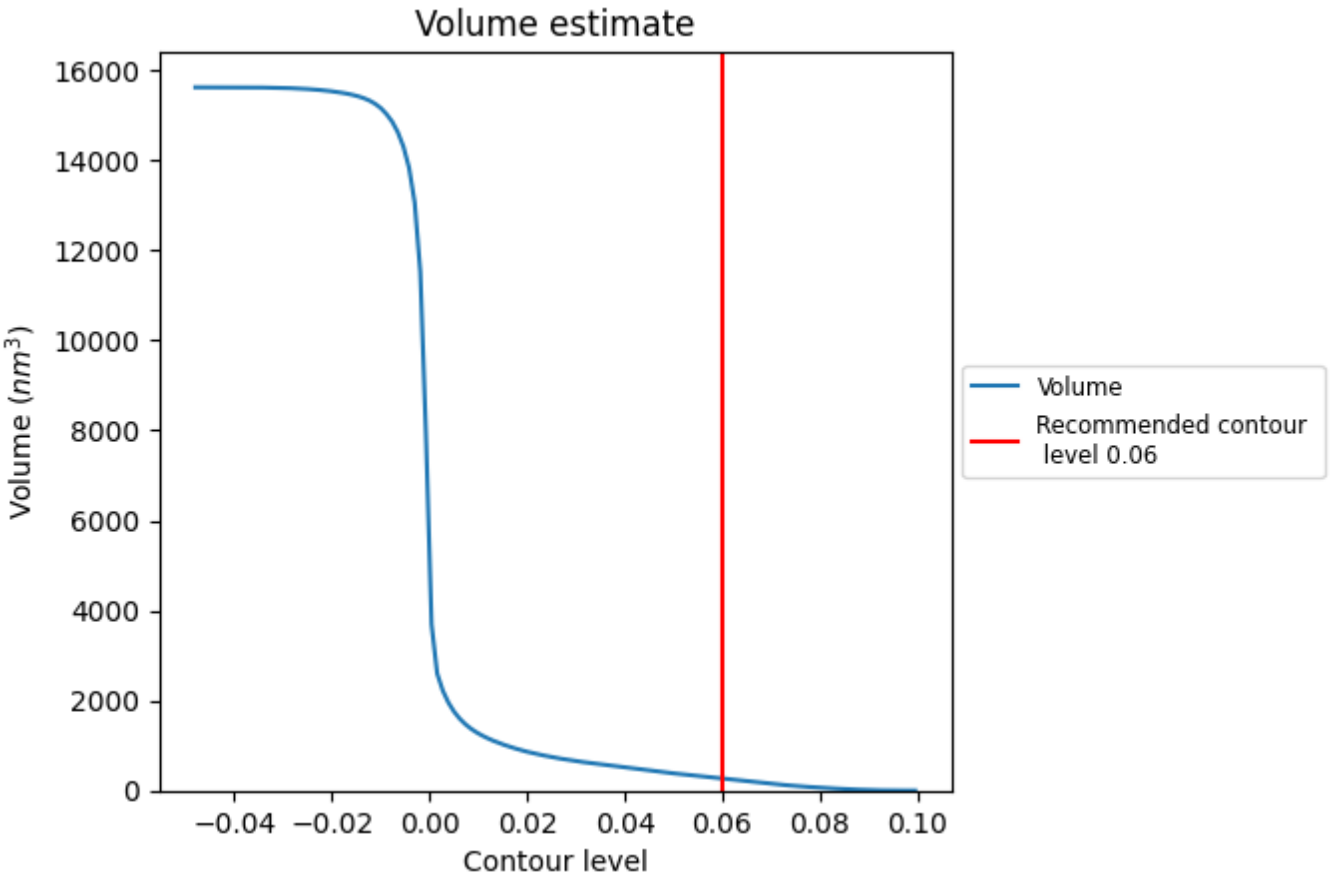
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

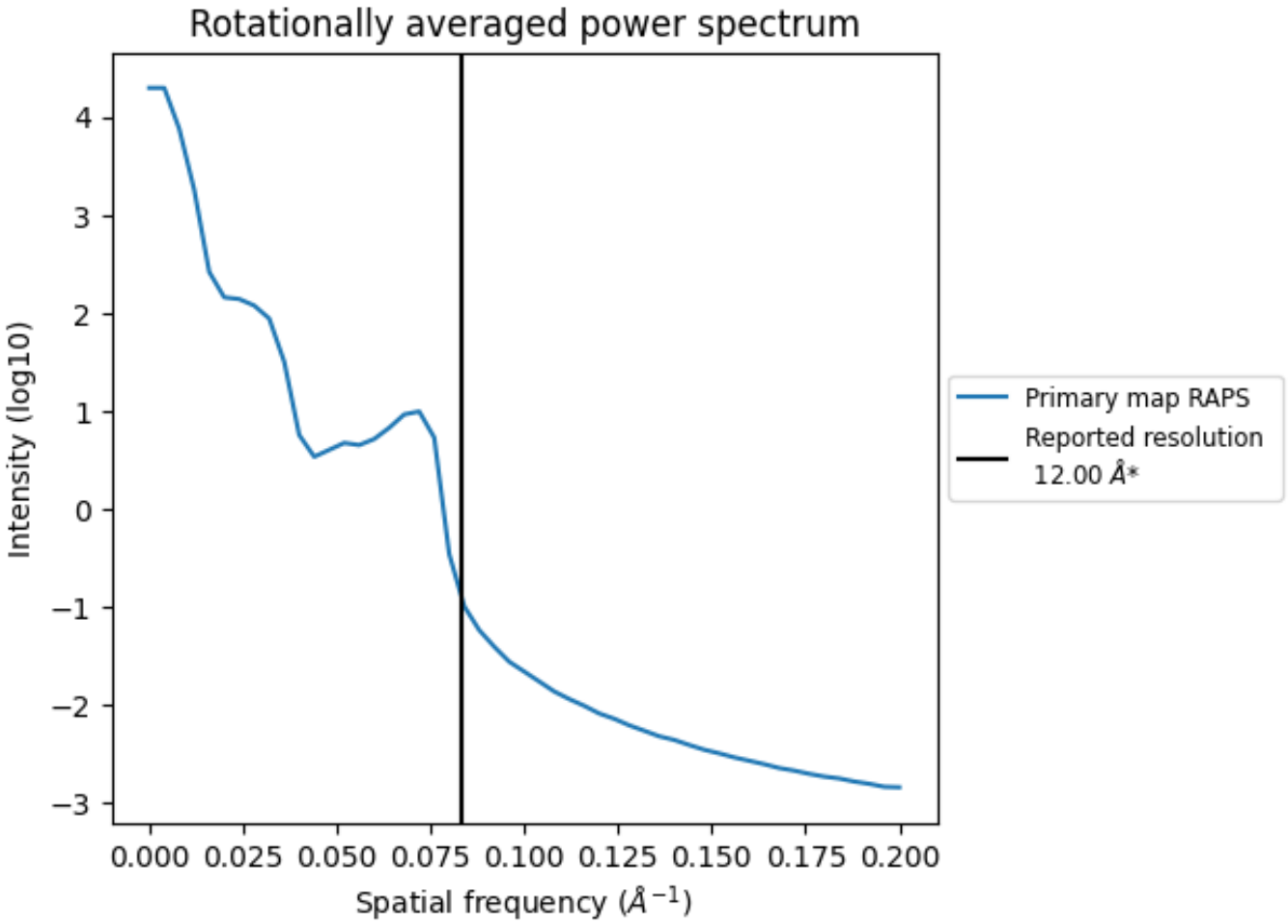
7.2 Volume estimate



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 242 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)



*Reported resolution corresponds to spatial frequency of 0.083 Å^{-1}

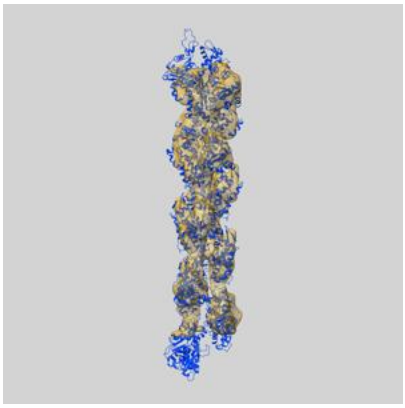
8 Fourier-Shell correlation (i)

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

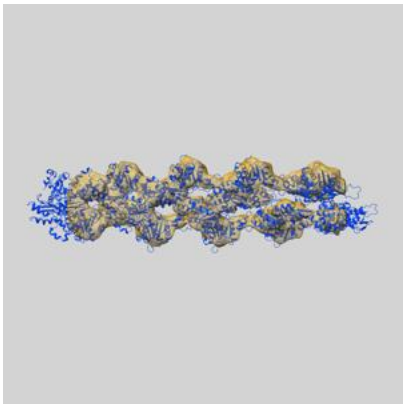
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6181 and PDB model 3J8K. Per-residue inclusion information can be found in section 3 on page 5.

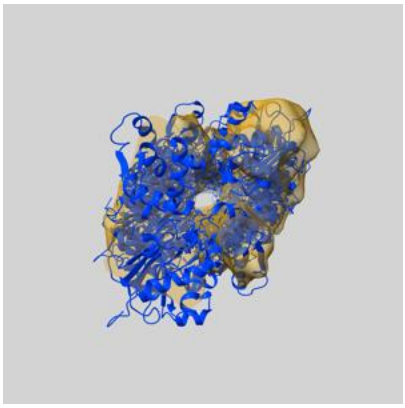
9.1 Map-model overlay



X



Y



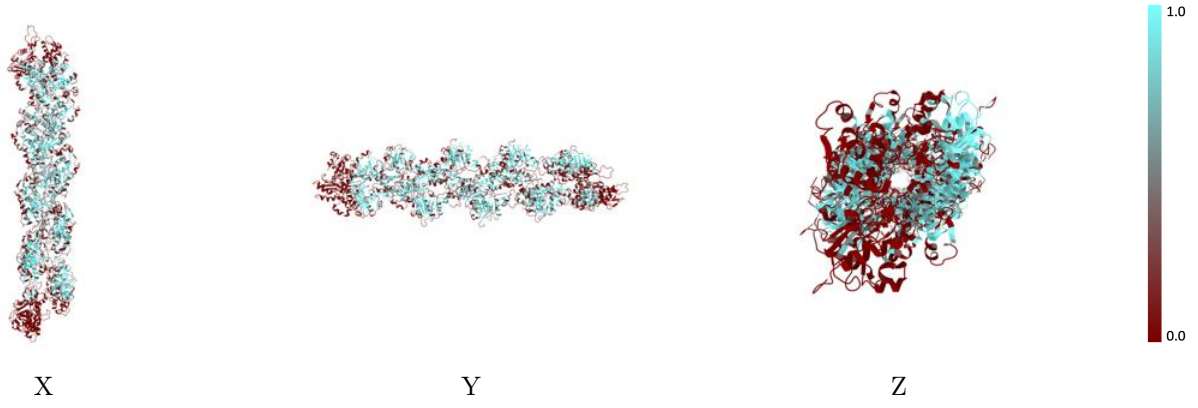
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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

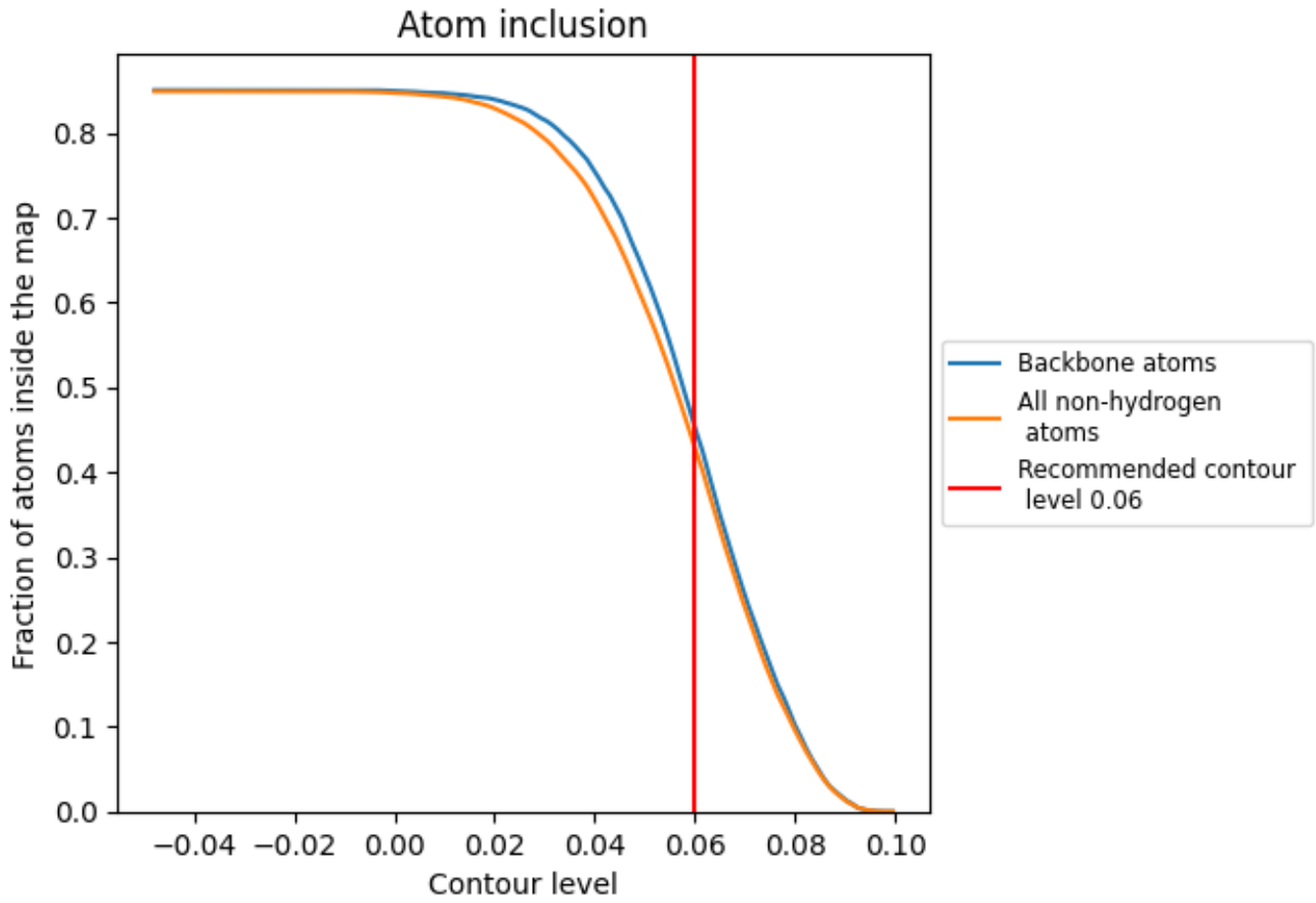
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 43% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4292	0.0560
A	0.0483	0.0070
B	0.4390	0.0530
C	0.5134	0.0730
D	0.5283	0.0710
E	0.5148	0.0740
F	0.5231	0.0690
G	0.5193	0.0750
H	0.5221	0.0710
I	0.4929	0.0560
J	0.1908	0.0150