



Full wwPDB EM Validation Report ⓘ

Jun 27, 2024 – 09:47 AM JST

PDB ID : 8JNS
EMDB ID : EMD-36450
Title : cryo-EM structure of a CED-4 hexamer
Authors : Li, Y.; Shi, Y.
Deposited on : 2023-06-06
Resolution : 4.20 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.dev92
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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

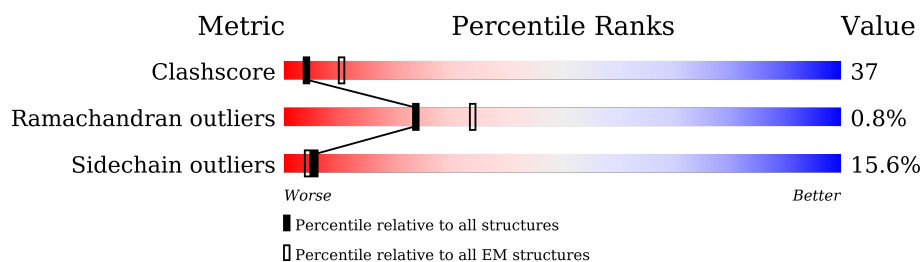
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	A	549	<div> <div>11%</div> <div>39%</div> <div>43%</div> <div>10%</div> <div>8%</div> </div>
1	B	549	<div> <div>6%</div> <div>38%</div> <div>45%</div> <div>8%</div> <div>8%</div> </div>
1	C	549	<div> <div>6%</div> <div>38%</div> <div>45%</div> <div>8%</div> <div>8%</div> </div>
1	D	549	<div> <div>30%</div> <div>35%</div> <div>6%</div> <div>29%</div> </div>
1	E	549	<div> <div>7%</div> <div>30%</div> <div>35%</div> <div>7%</div> <div>29%</div> </div>
1	F	549	<div> <div>30%</div> <div>34%</div> <div>8%</div> <div>29%</div> </div>
1	G	549	<div> <div>13%</div> <div>8%</div> <div>8%</div> <div>82%</div> </div>
1	H	549	<div> <div>16%</div> <div>7%</div> <div>9%</div> <div>82%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	549	<p>14% 7% 9% 82%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24168 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 Cell death protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	503	Total	C	N	O	S	0	0
			4039	2575	676	759	29		
1	B	503	Total	C	N	O	S	0	0
			4039	2575	676	759	29		
1	C	503	Total	C	N	O	S	0	0
			4039	2575	676	759	29		
1	D	392	Total	C	N	O	S	0	0
			3123	1992	519	587	25		
1	E	392	Total	C	N	O	S	0	0
			3123	1992	519	587	25		
1	F	392	Total	C	N	O	S	0	0
			3123	1992	519	587	25		
1	G	100	Total	C	N	O	S	0	0
			830	525	142	159	4		
1	H	100	Total	C	N	O	S	0	0
			830	525	142	159	4		
1	I	100	Total	C	N	O	S	0	0
			830	525	142	159	4		

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

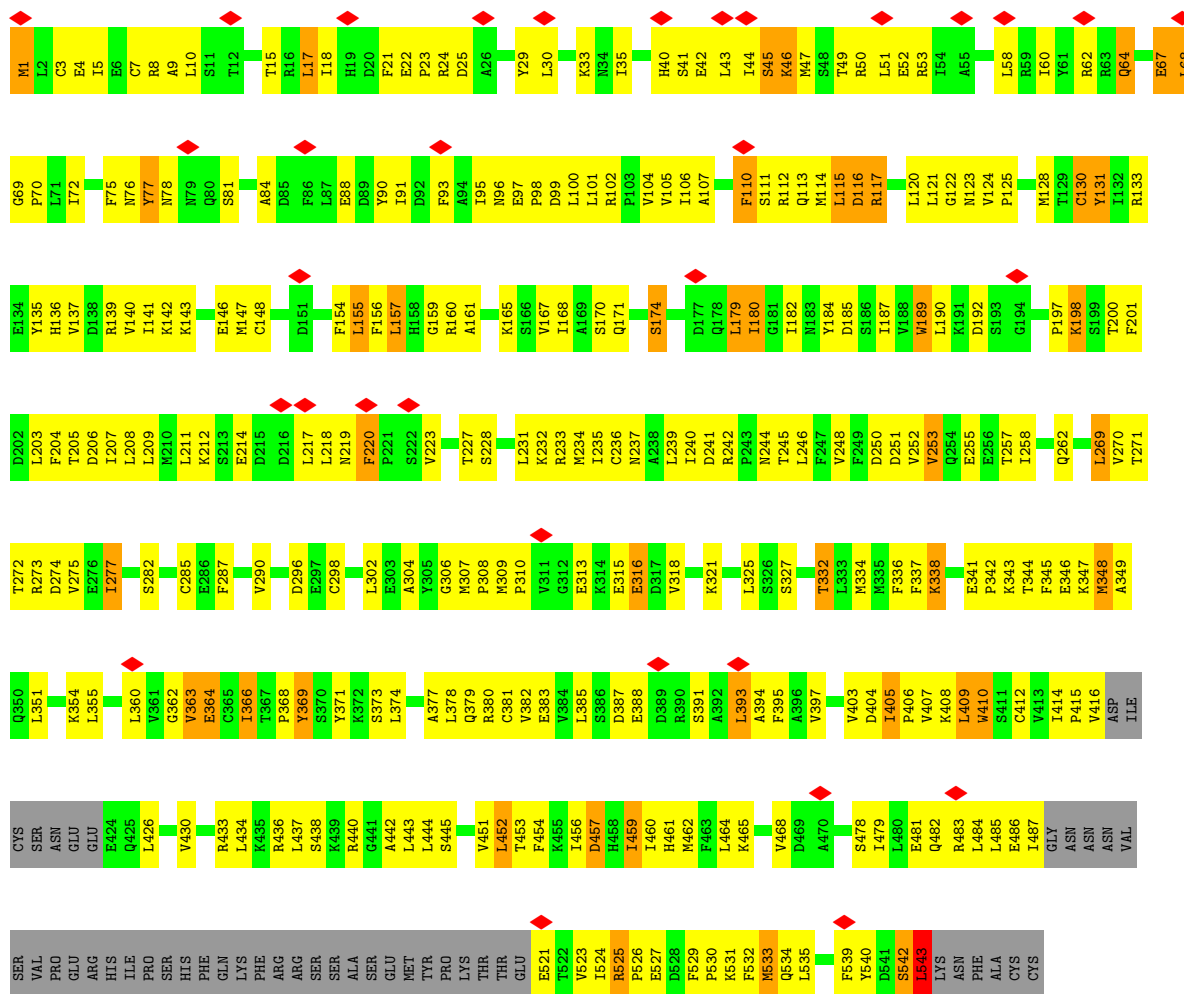
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	
2	B	1	Total	Mg	0
			1	1	
2	C	1	Total	Mg	0
			1	1	
2	D	1	Total	Mg	0
			1	1	
2	E	1	Total	Mg	0
			1	1	

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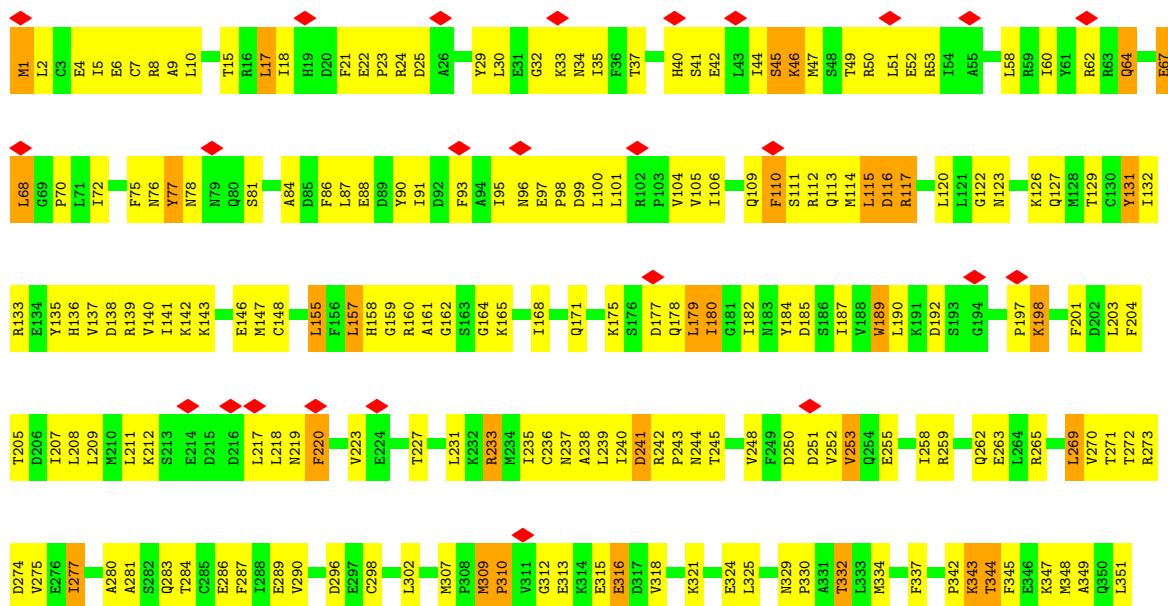
Mol	Chain	Residues	Atoms	AltConf
2	F	1	Total Mg 1 1	0

- # ATP

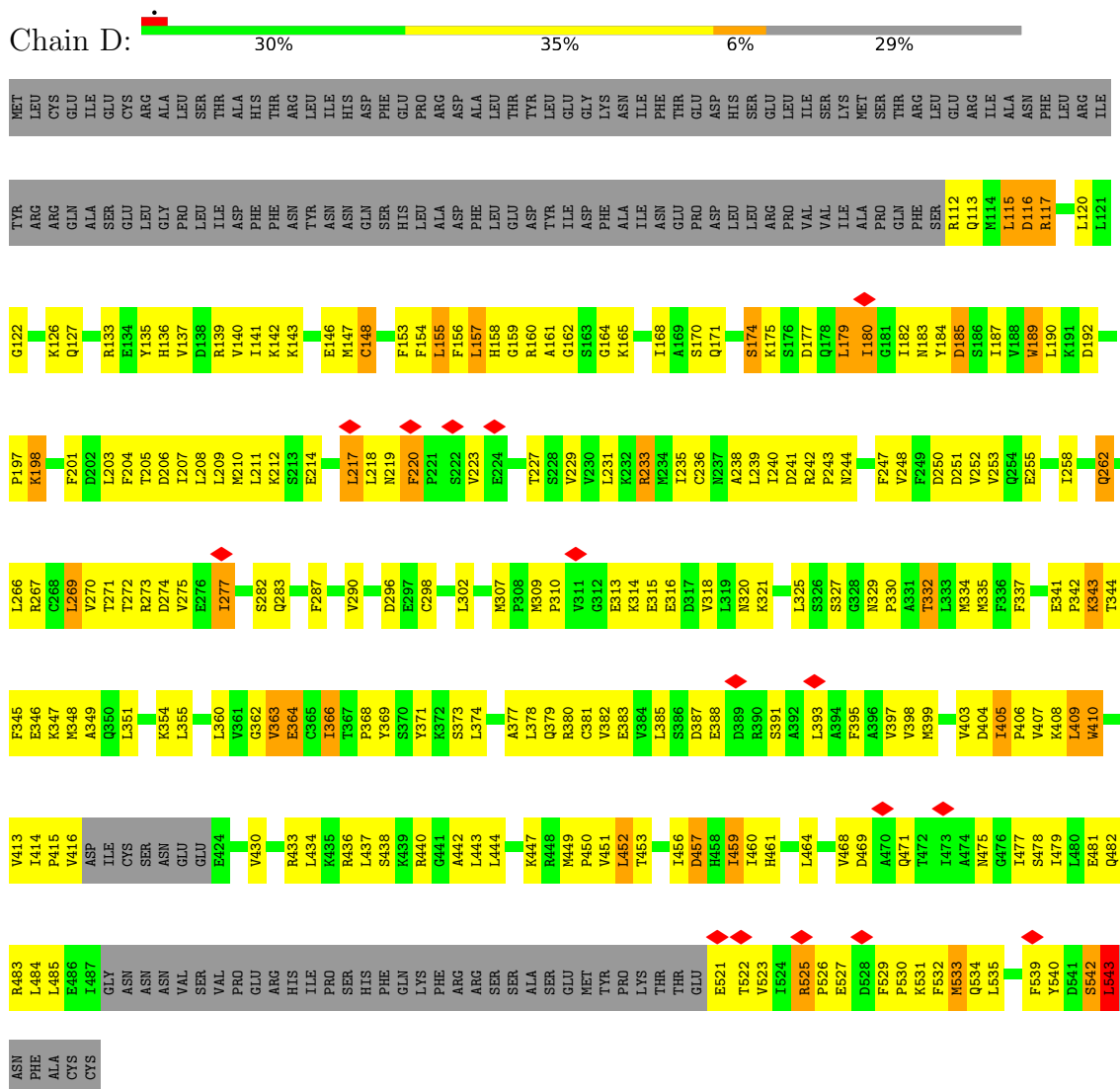
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0



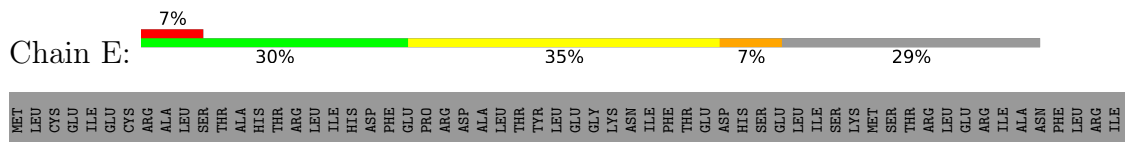
• Molecule 1: Cell death protein 4

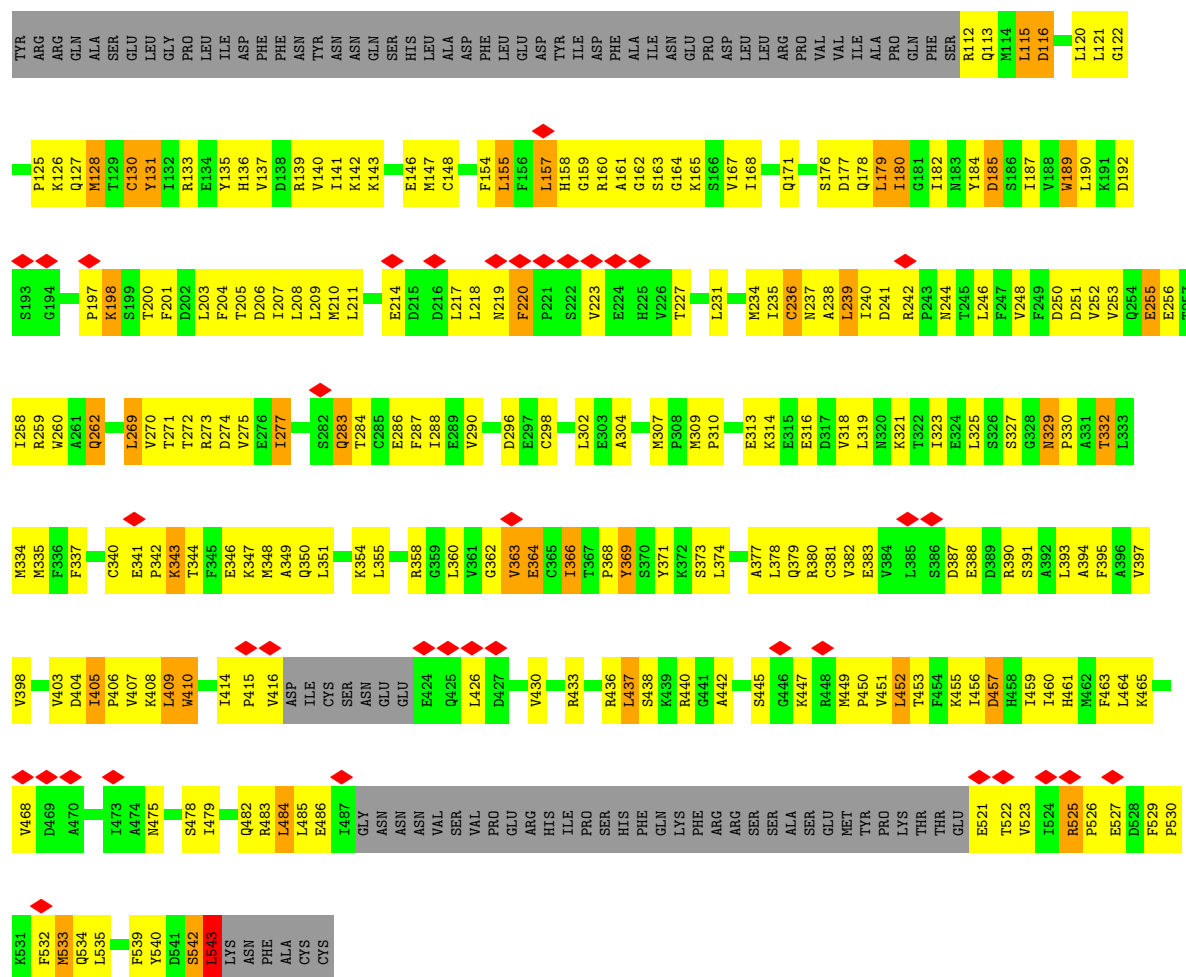


- Molecule 1: Cell death protein 4

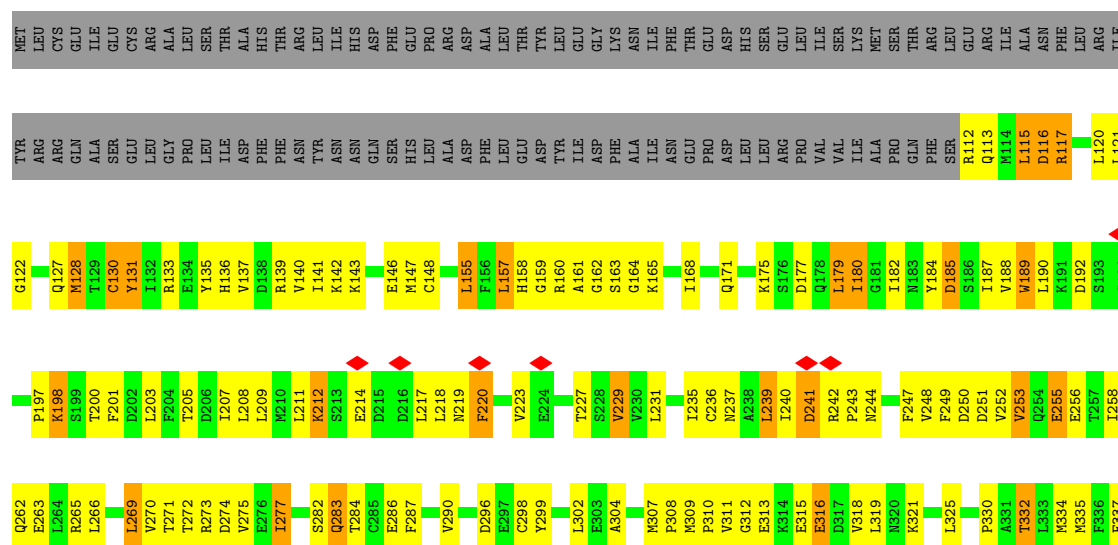


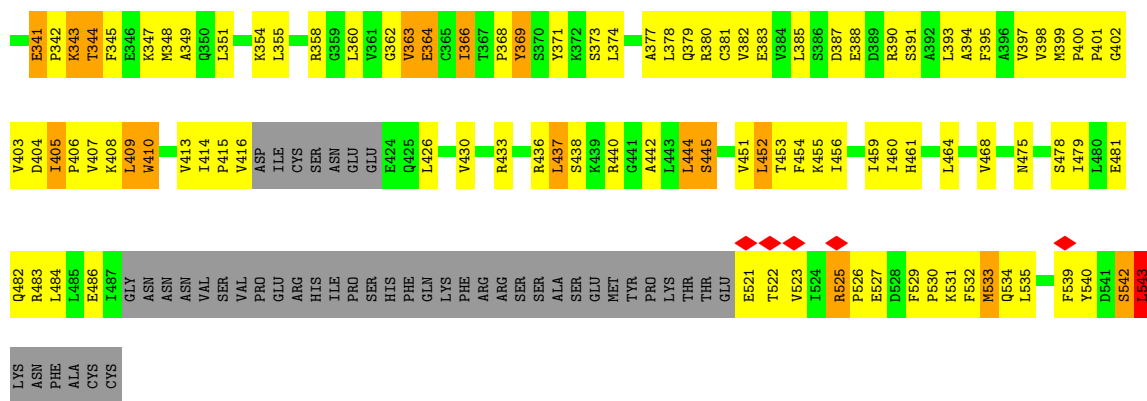
- Molecule 1: Cell death protein 4



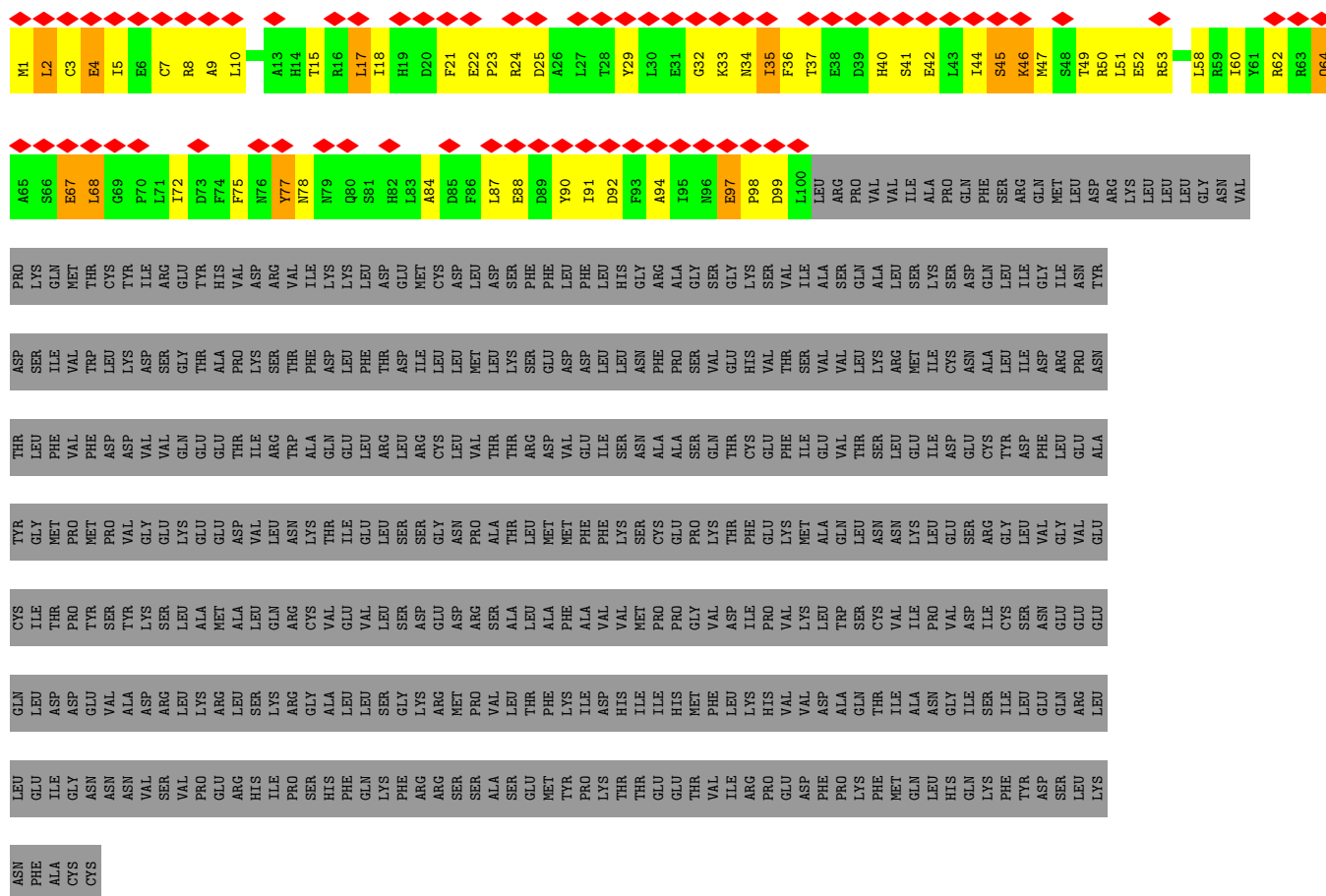


• Molecule 1: Cell death protein 4

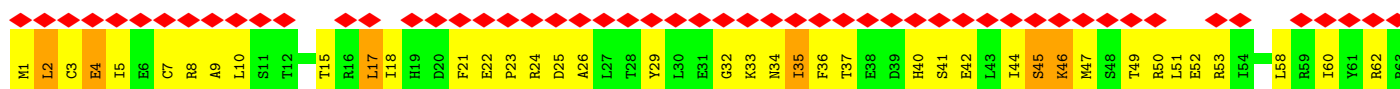




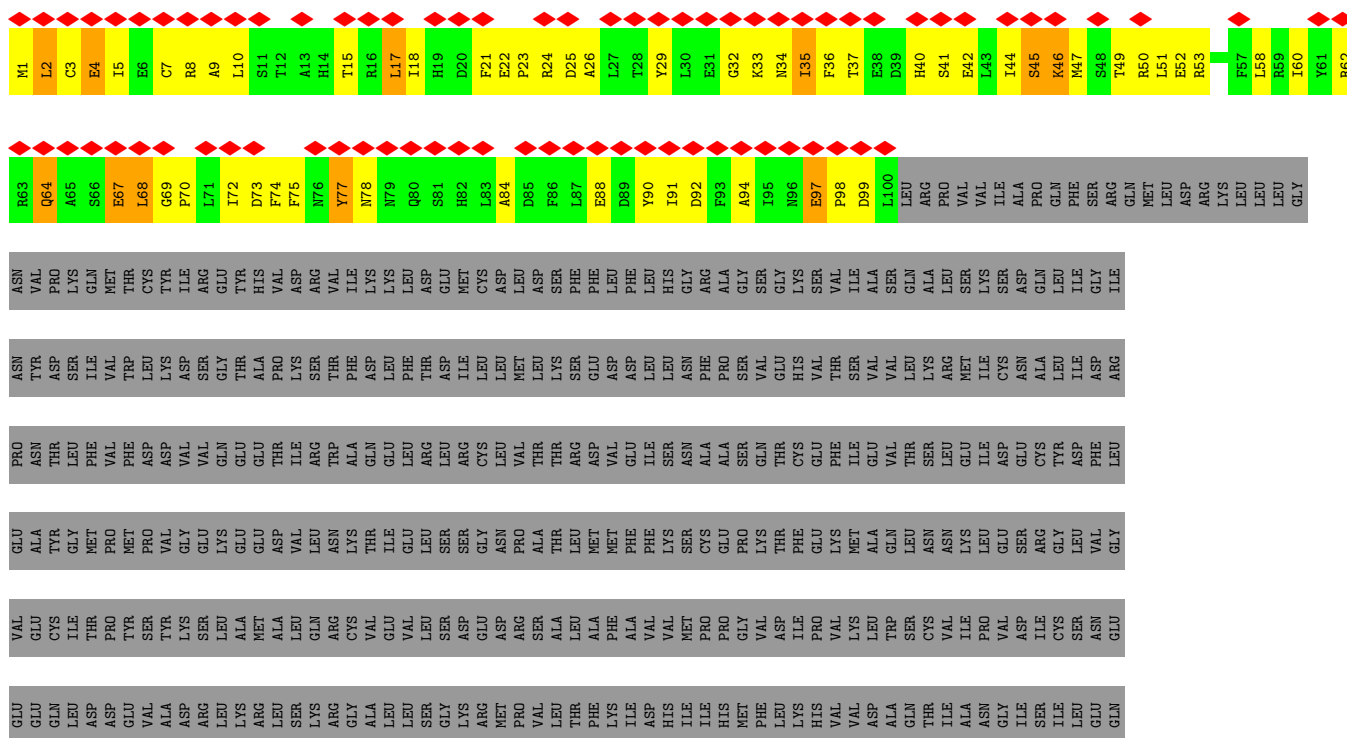
• Molecule 1: Cell death protein 4



• Molecule 1: Cell death protein 4



- Molecule 1: Cell death protein 4



ARG
LEU
LEU
GLU
ILE
ILE
GLY
ASN
ASN
ASN
VAL
SER
VAL
PRO
GLU
ARG
HIS
ILE
PRO
SER
HIS
PHE
GLN
LYS
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ARG
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SER
SER
ALA
SER
GLU
MET
TYR
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ASP
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GLN
LEU
HIS
GLN
LYS
PHE
TYR
ASP
SER

LEU
LYS
ASN
PHE
ALA
CYS
CYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125140	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.46	0/4113	0.64	2/5558 (0.0%)
1	B	0.43	0/4113	0.60	2/5558 (0.0%)
1	C	0.43	0/4113	0.61	2/5558 (0.0%)
1	D	0.45	0/3176	0.63	2/4288 (0.0%)
1	E	0.45	0/3176	0.61	2/4288 (0.0%)
1	F	0.44	0/3176	0.61	2/4288 (0.0%)
1	G	0.38	0/847	0.52	0/1144
1	H	0.38	0/847	0.52	0/1144
1	I	0.38	0/847	0.52	0/1144
All	All	0.44	0/24408	0.61	12/32970 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	409	LEU	CA-CB-CG	5.45	127.82	115.30
1	B	409	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	409	LEU	CA-CB-CG	5.43	127.79	115.30
1	E	409	LEU	CA-CB-CG	5.43	127.79	115.30
1	F	409	LEU	CA-CB-CG	5.43	127.78	115.30
1	F	543	LEU	CA-CB-CG	5.17	127.18	115.30
1	D	543	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	543	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	543	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	543	LEU	CA-CB-CG	5.15	127.15	115.30
1	E	543	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4039	0	4066	308	0
1	B	4039	0	4066	316	0
1	C	4039	0	4066	331	0
1	D	3123	0	3171	242	0
1	E	3123	0	3171	214	0
1	F	3123	0	3171	250	0
1	G	830	0	800	72	0
1	H	830	0	800	65	0
1	I	830	0	800	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	12	6	0
3	B	31	0	12	5	0
3	C	31	0	12	5	0
3	D	31	0	12	6	0
3	E	31	0	12	6	0
3	F	31	0	12	6	0
All	All	24168	0	24183	1785	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 37.

All (1785) 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:B:97:GLU:CD	1:I:51:LEU:CD1	1.74	1.53
1:B:97:GLU:CD	1:I:51:LEU:HD12	1.10	1.47
1:C:97:GLU:CD	1:G:51:LEU:HD12	1.28	1.46
1:C:97:GLU:CD	1:G:51:LEU:CD1	1.80	1.44
1:C:97:GLU:OE2	1:G:51:LEU:HD12	1.21	1.29
1:B:97:GLU:OE2	1:I:51:LEU:HD12	1.30	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:CZ	1:F:240:ILE:HG22	1.70	1.21
1:B:97:GLU:CG	1:I:51:LEU:CD1	2.19	1.20
1:B:1:MET:SD	1:F:117:ARG:HG3	1.83	1.18
1:C:117:ARG:NH1	1:F:240:ILE:HG22	1.57	1.18
1:C:117:ARG:NH2	1:F:240:ILE:HG22	1.57	1.18
1:A:236:CYS:HB2	1:D:120:LEU:CD2	1.77	1.13
1:D:208:LEU:HD23	1:D:235:ILE:HA	1.30	1.11
1:C:120:LEU:HD21	1:F:236:CYS:HB2	1.30	1.09
1:A:236:CYS:CB	1:D:120:LEU:HD21	1.83	1.08
1:C:97:GLU:CD	1:G:51:LEU:HD13	1.67	1.06
1:B:97:GLU:CG	1:I:51:LEU:HD12	1.83	1.05
1:C:236:CYS:HB2	1:E:120:LEU:HD21	1.30	1.05
1:B:97:GLU:HG3	1:I:51:LEU:CD1	1.84	1.04
1:C:117:ARG:HH12	1:F:240:ILE:CG2	1.71	1.04
1:C:97:GLU:CG	1:G:51:LEU:CD1	2.34	1.04
1:C:395:PHE:HB3	1:C:413:VAL:HB	1.34	1.04
1:B:236:CYS:HB2	1:F:120:LEU:HD21	1.35	1.03
1:B:97:GLU:CD	1:I:51:LEU:HD13	1.75	1.02
1:A:240:ILE:HG22	1:D:117:ARG:HH12	1.25	1.01
1:B:208:LEU:HD23	1:B:235:ILE:HA	1.41	1.01
1:A:41:SER:O	1:A:45:SER:HB3	1.61	1.01
1:B:93:PHE:HE2	1:B:100:LEU:HD23	1.24	1.00
1:C:93:PHE:HE2	1:C:100:LEU:HD23	1.24	1.00
1:A:93:PHE:HE2	1:A:100:LEU:HD23	1.24	1.00
1:C:41:SER:O	1:C:45:SER:HB3	1.61	1.00
1:G:41:SER:O	1:G:45:SER:HB3	1.62	1.00
1:B:41:SER:O	1:B:45:SER:HB3	1.61	1.00
1:H:41:SER:O	1:H:45:SER:HB3	1.62	0.99
1:I:41:SER:O	1:I:45:SER:HB3	1.62	0.99
1:F:208:LEU:HD23	1:F:235:ILE:HA	1.46	0.95
1:C:97:GLU:OE1	1:G:51:LEU:HD13	1.65	0.95
1:B:97:GLU:OE1	1:I:51:LEU:HD13	1.68	0.94
1:C:117:ARG:NH1	1:F:240:ILE:CG2	2.30	0.93
1:B:8:ARG:HG2	1:B:8:ARG:HH11	1.33	0.93
1:B:240:ILE:HG22	1:F:117:ARG:HH12	1.34	0.93
1:B:121:LEU:HD22	1:D:233:ARG:NE	1.85	0.92
1:C:117:ARG:HH22	1:F:240:ILE:CG2	1.81	0.92
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.33	0.91
1:C:117:ARG:HH22	1:F:240:ILE:HG22	1.25	0.91
1:B:123:ASN:OD1	1:D:229:VAL:HG23	1.71	0.91
1:C:120:LEU:HD21	1:F:236:CYS:CB	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.33	0.91
1:A:443:LEU:HD23	1:A:460:ILE:HD11	1.53	0.91
1:G:8:ARG:HG2	1:G:8:ARG:HH11	1.35	0.90
1:B:97:GLU:OE1	1:I:51:LEU:CD1	2.17	0.90
1:I:8:ARG:HG2	1:I:8:ARG:HH11	1.35	0.90
1:A:93:PHE:CE2	1:A:100:LEU:HD23	2.07	0.90
1:A:236:CYS:HB2	1:D:120:LEU:HD21	0.92	0.90
1:B:93:PHE:CE2	1:B:100:LEU:HD23	2.07	0.89
1:C:93:PHE:CE2	1:C:100:LEU:HD23	2.07	0.89
1:C:342:PRO:HG2	1:C:347:LYS:HG3	1.52	0.89
1:D:443:LEU:HD23	1:D:460:ILE:HD11	1.53	0.89
1:H:8:ARG:HG2	1:H:8:ARG:HH11	1.35	0.89
1:H:47:MET:HB2	1:H:53:ARG:HG3	1.56	0.88
1:A:212:LYS:HE2	1:A:212:LYS:HA	1.54	0.88
1:C:158:HIS:CE1	1:C:289:GLU:HB2	2.07	0.88
1:F:398:VAL:HG21	1:F:413:VAL:HG11	1.53	0.88
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.54	0.88
1:A:240:ILE:HA	1:D:117:ARG:HH22	1.35	0.88
1:A:158:HIS:CE1	1:A:289:GLU:HB2	2.07	0.88
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.14	0.88
1:I:47:MET:HB2	1:I:53:ARG:HG3	1.56	0.88
1:B:7:CYS:SG	1:B:62:ARG:HD3	2.14	0.88
1:A:158:HIS:HE1	1:A:289:GLU:HB2	1.38	0.88
1:A:47:MET:HB2	1:A:53:ARG:HG3	1.55	0.87
1:C:47:MET:HB2	1:C:53:ARG:HG3	1.55	0.87
1:B:212:LYS:HA	1:B:212:LYS:HE2	1.54	0.87
1:C:90:TYR:HE2	1:C:106:ILE:HD11	1.40	0.87
1:B:97:GLU:HG3	1:I:51:LEU:HD11	1.55	0.87
1:F:208:LEU:HB2	1:F:235:ILE:HG12	1.55	0.87
1:F:342:PRO:HG2	1:F:347:LYS:HG3	1.57	0.86
1:B:240:ILE:HA	1:F:117:ARG:HH22	1.41	0.86
1:C:97:GLU:HG3	1:G:51:LEU:CD1	2.03	0.86
1:C:158:HIS:HE1	1:C:289:GLU:HB2	1.38	0.86
1:C:212:LYS:HE2	1:C:212:LYS:HA	1.54	0.86
1:B:47:MET:HB2	1:B:53:ARG:HG3	1.55	0.86
1:C:7:CYS:SG	1:C:62:ARG:HD3	2.14	0.86
1:C:117:ARG:NH2	1:F:240:ILE:CG2	2.38	0.86
1:H:7:CYS:SG	1:H:62:ARG:HD3	2.16	0.85
1:G:7:CYS:SG	1:G:62:ARG:HD3	2.16	0.85
1:G:47:MET:HB2	1:G:53:ARG:HG3	1.56	0.85
1:A:342:PRO:HG2	1:A:347:LYS:HG3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HH12	1:D:240:ILE:HG22	1.39	0.84
1:E:135:TYR:O	1:E:139:ARG:HG3	1.78	0.84
1:I:7:CYS:SG	1:I:62:ARG:HD3	2.16	0.84
1:A:30:LEU:HD22	1:A:35:ILE:HG13	1.59	0.84
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.43	0.83
1:G:75:PHE:HB2	1:G:84:ALA:HB2	1.60	0.83
1:H:75:PHE:HB2	1:H:84:ALA:HB2	1.60	0.83
1:D:135:TYR:O	1:D:139:ARG:HG3	1.78	0.83
1:C:135:TYR:O	1:C:139:ARG:HG3	1.78	0.83
1:B:135:TYR:O	1:B:139:ARG:HG3	1.78	0.83
1:A:135:TYR:O	1:A:139:ARG:HG3	1.78	0.83
1:A:160:ARG:HH21	1:A:459:ILE:HD12	1.44	0.83
1:A:127:GLN:HB2	1:A:171:GLN:HG2	1.58	0.82
1:A:240:ILE:HG22	1:D:117:ARG:NH1	1.93	0.82
1:B:1:MET:SD	1:F:117:ARG:CG	2.66	0.82
1:F:135:TYR:O	1:F:139:ARG:HG3	1.78	0.82
1:A:102:ARG:HA	1:A:106:ILE:HB	1.60	0.82
1:A:398:VAL:HG21	1:A:413:VAL:HG11	1.61	0.82
1:B:44:ILE:HD11	1:B:60:ILE:HD12	1.61	0.82
1:E:366:ILE:HD12	1:E:366:ILE:H	1.45	0.82
1:E:197:PRO:HD2	1:E:198:LYS:HE2	1.62	0.82
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.60	0.81
1:C:44:ILE:HD11	1:C:60:ILE:HD12	1.61	0.81
1:C:75:PHE:HB2	1:C:84:ALA:HB2	1.60	0.81
1:A:44:ILE:O	1:A:53:ARG:HG2	1.80	0.81
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.62	0.81
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.62	0.81
1:I:75:PHE:HB2	1:I:84:ALA:HB2	1.60	0.81
1:E:141:ILE:HD13	1:E:176:SER:HB2	1.60	0.81
1:F:197:PRO:HD2	1:F:198:LYS:HE2	1.62	0.81
1:F:366:ILE:H	1:F:366:ILE:HD12	1.45	0.81
1:A:366:ILE:H	1:A:366:ILE:HD12	1.45	0.81
1:C:44:ILE:O	1:C:53:ARG:HG2	1.80	0.81
1:B:366:ILE:HD12	1:B:366:ILE:H	1.45	0.80
1:C:97:GLU:CG	1:G:51:LEU:HD12	2.07	0.80
1:C:366:ILE:H	1:C:366:ILE:HD12	1.45	0.80
1:D:197:PRO:HD2	1:D:198:LYS:HE2	1.62	0.80
1:D:366:ILE:H	1:D:366:ILE:HD12	1.45	0.80
1:C:197:PRO:HD2	1:C:198:LYS:HE2	1.62	0.80
1:D:115:LEU:HD21	1:D:180:ILE:HB	1.63	0.80
1:B:44:ILE:O	1:B:53:ARG:HG2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HD21	1:C:180:ILE:HB	1.63	0.80
1:C:127:GLN:HB2	1:C:171:GLN:HG2	1.64	0.80
1:C:97:GLU:OE1	1:G:51:LEU:CD1	2.25	0.80
1:C:255:GLU:HA	1:C:258:ILE:HD13	1.62	0.80
1:A:44:ILE:HD11	1:A:60:ILE:HD12	1.61	0.80
1:B:342:PRO:HG2	1:B:347:LYS:HG3	1.62	0.80
1:F:401:PRO:HA	1:F:456:ILE:HG23	1.62	0.80
1:B:115:LEU:HD21	1:B:180:ILE:HB	1.64	0.79
1:B:255:GLU:HA	1:B:258:ILE:HD13	1.64	0.79
1:F:255:GLU:HA	1:F:258:ILE:HD13	1.65	0.79
1:D:262:GLN:HE21	1:D:283:GLN:HB2	1.46	0.79
1:C:313:GLU:O	1:C:316:GLU:HG3	1.82	0.79
1:C:117:ARG:HH12	1:F:240:ILE:HG22	1.25	0.79
1:D:456:ILE:HG13	1:D:460:ILE:CG2	2.13	0.79
1:F:115:LEU:HD21	1:F:180:ILE:HB	1.63	0.79
1:A:456:ILE:HG13	1:A:460:ILE:CG2	2.13	0.79
1:C:117:ARG:HH22	1:F:240:ILE:HA	1.46	0.78
1:E:115:LEU:HD21	1:E:180:ILE:HB	1.63	0.78
1:F:464:LEU:O	1:F:468:VAL:HG22	1.82	0.78
1:C:117:ARG:HH22	1:F:240:ILE:CB	1.97	0.78
1:C:190:LEU:HD12	1:C:207:ILE:HG12	1.66	0.78
1:B:456:ILE:HG13	1:B:460:ILE:CG2	2.13	0.77
1:A:8:ARG:HE	1:A:244:ASN:HD22	1.31	0.77
1:C:452:LEU:HD23	1:C:452:LEU:H	1.50	0.77
1:D:452:LEU:HD23	1:D:452:LEU:H	1.50	0.77
1:B:120:LEU:HD21	1:D:236:CYS:CB	2.15	0.76
1:B:121:LEU:HB3	1:D:233:ARG:HE	1.51	0.76
1:E:452:LEU:HD23	1:E:452:LEU:H	1.50	0.76
1:G:44:ILE:O	1:G:53:ARG:HG2	1.86	0.76
1:A:452:LEU:HD23	1:A:452:LEU:H	1.50	0.76
1:B:452:LEU:HD23	1:B:452:LEU:H	1.50	0.76
1:H:44:ILE:HD11	1:H:60:ILE:HD12	1.68	0.76
1:E:456:ILE:HD11	1:E:461:HIS:HA	1.68	0.76
1:I:44:ILE:O	1:I:53:ARG:HG2	1.86	0.76
1:D:342:PRO:HG2	1:D:347:LYS:HG3	1.67	0.75
1:F:452:LEU:H	1:F:452:LEU:HD23	1.50	0.75
1:B:90:TYR:HE2	1:B:106:ILE:HD11	1.51	0.75
1:I:44:ILE:HD11	1:I:60:ILE:HD12	1.68	0.75
1:D:398:VAL:HG21	1:D:413:VAL:HG11	1.67	0.75
1:H:44:ILE:O	1:H:53:ARG:HG2	1.86	0.75
1:B:30:LEU:HD22	1:B:35:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ILE:HD11	1:G:60:ILE:HD12	1.68	0.75
1:C:111:SER:HB3	1:C:114:MET:SD	2.26	0.74
1:C:117:ARG:HH22	1:F:240:ILE:CA	1.98	0.74
1:B:236:CYS:HB2	1:F:120:LEU:CD2	2.17	0.74
1:D:415:PRO:O	1:D:416:VAL:HG23	1.88	0.74
1:A:415:PRO:O	1:A:416:VAL:HG23	1.88	0.74
1:C:415:PRO:O	1:C:416:VAL:HG23	1.88	0.74
1:F:364:GLU:HB2	1:F:373:SER:HB3	1.70	0.74
1:F:415:PRO:O	1:F:416:VAL:HG23	1.88	0.74
1:A:72:ILE:HG23	1:A:84:ALA:HB1	1.68	0.74
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.70	0.74
1:E:364:GLU:HB2	1:E:373:SER:HB3	1.70	0.74
1:E:415:PRO:O	1:E:416:VAL:HG23	1.88	0.74
1:A:406:PRO:HA	1:A:453:THR:HG22	1.70	0.73
1:D:364:GLU:HB2	1:D:373:SER:HB3	1.70	0.73
1:I:40:HIS:ND1	1:I:60:ILE:HD13	2.04	0.73
1:B:252:VAL:HG11	1:B:258:ILE:HD11	1.69	0.73
1:G:40:HIS:ND1	1:G:60:ILE:HD13	2.04	0.73
1:B:313:GLU:O	1:B:316:GLU:HG3	1.89	0.73
1:C:364:GLU:HB2	1:C:373:SER:HB3	1.70	0.73
1:E:406:PRO:HA	1:E:453:THR:HG22	1.70	0.73
1:B:120:LEU:HD21	1:D:236:CYS:SG	2.28	0.73
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.24	0.73
1:C:135:TYR:CE1	1:C:139:ARG:HD2	2.24	0.73
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.70	0.72
1:D:406:PRO:HA	1:D:453:THR:HG22	1.70	0.72
1:A:529:PHE:N	1:A:530:PRO:HD3	2.04	0.72
1:C:406:PRO:HA	1:C:453:THR:HG22	1.70	0.72
1:D:135:TYR:CE1	1:D:139:ARG:HD2	2.24	0.72
1:H:40:HIS:ND1	1:H:60:ILE:HD13	2.04	0.72
1:B:406:PRO:HA	1:B:453:THR:HG22	1.70	0.72
1:B:529:PHE:N	1:B:530:PRO:HD3	2.05	0.72
1:A:159:GLY:N	1:A:165:LYS:HD3	2.04	0.72
1:B:415:PRO:O	1:B:416:VAL:HG23	1.88	0.72
1:D:397:VAL:HG22	1:D:464:LEU:HB3	1.71	0.72
1:F:135:TYR:CE1	1:F:139:ARG:HD2	2.24	0.72
1:E:529:PHE:N	1:E:530:PRO:HD3	2.04	0.72
1:F:529:PHE:N	1:F:530:PRO:HD3	2.05	0.72
1:E:127:GLN:HB2	1:E:171:GLN:HG2	1.70	0.72
1:D:529:PHE:N	1:D:530:PRO:HD3	2.04	0.72
1:E:158:HIS:NE2	1:E:287:PHE:HB3	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:MET:HE2	1:D:217:LEU:HD12	1.72	0.71
1:B:327:SER:HB2	1:B:459:ILE:HD11	1.71	0.71
1:E:135:TYR:CE1	1:E:139:ARG:HD2	2.24	0.71
1:E:484:LEU:HD11	1:E:533:MET:HG2	1.72	0.71
1:E:115:LEU:HD11	1:E:177:ASP:HA	1.71	0.71
1:B:111:SER:HB3	1:B:114:MET:SD	2.31	0.71
1:C:208:LEU:HB2	1:C:235:ILE:HG12	1.71	0.71
1:A:283:GLN:HG2	1:A:284:THR:H	1.54	0.71
1:C:252:VAL:HG11	1:C:258:ILE:HD11	1.71	0.71
1:I:64:GLN:HE21	1:I:64:GLN:HA	1.56	0.71
1:E:184:TYR:HA	1:E:244:ASN:HB3	1.71	0.71
1:G:64:GLN:HA	1:G:64:GLN:HE21	1.56	0.71
1:C:159:GLY:N	1:C:165:LYS:HD3	2.05	0.71
1:C:529:PHE:HB3	1:C:532:PHE:CE1	2.25	0.71
1:A:135:TYR:CE1	1:A:139:ARG:HD2	2.24	0.71
1:E:393:LEU:HD21	1:E:464:LEU:HD22	1.72	0.71
1:B:33:LYS:HD3	1:B:70:PRO:HB3	1.71	0.71
1:D:534:GLN:HA	1:D:534:GLN:HE21	1.56	0.70
1:H:64:GLN:HA	1:H:64:GLN:HE21	1.56	0.70
1:E:534:GLN:HE21	1:E:534:GLN:HA	1.56	0.70
1:A:534:GLN:HA	1:A:534:GLN:HE21	1.56	0.70
1:C:137:VAL:O	1:C:141:ILE:HG13	1.92	0.70
1:D:137:VAL:O	1:D:141:ILE:HG13	1.92	0.70
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.72	0.70
1:A:542:SER:C	1:A:543:LEU:HD22	2.12	0.70
1:B:542:SER:C	1:B:543:LEU:HD22	2.12	0.70
1:B:137:VAL:O	1:B:141:ILE:HG13	1.92	0.70
1:D:542:SER:C	1:D:543:LEU:HD22	2.12	0.70
1:F:208:LEU:CD2	1:F:235:ILE:HA	2.19	0.70
1:C:33:LYS:HD3	1:C:70:PRO:HB3	1.72	0.70
1:C:117:ARG:NH2	1:F:240:ILE:HA	2.06	0.70
1:C:542:SER:C	1:C:543:LEU:HD22	2.12	0.70
1:E:137:VAL:O	1:E:141:ILE:HG13	1.92	0.70
1:F:310:PRO:HA	1:F:345:PHE:CZ	2.27	0.70
1:A:40:HIS:ND1	1:A:60:ILE:HD13	2.07	0.69
1:E:176:SER:HB3	1:E:179:LEU:HD22	1.74	0.69
1:F:534:GLN:HA	1:F:534:GLN:HE21	1.56	0.69
1:B:393:LEU:HD23	1:B:393:LEU:C	2.12	0.69
1:C:529:PHE:N	1:C:530:PRO:HD3	2.07	0.69
1:A:137:VAL:O	1:A:141:ILE:HG13	1.92	0.69
1:B:534:GLN:HA	1:B:534:GLN:HE21	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:TYR:HA	1:D:244:ASN:HB3	1.74	0.69
1:F:137:VAL:O	1:F:141:ILE:HG13	1.92	0.69
1:F:542:SER:C	1:F:543:LEU:HD22	2.12	0.69
1:B:40:HIS:ND1	1:B:60:ILE:HD13	2.07	0.69
1:E:542:SER:C	1:E:543:LEU:HD22	2.12	0.69
1:C:534:GLN:HE21	1:C:534:GLN:HA	1.56	0.69
1:I:4:GLU:O	1:I:8:ARG:HB2	1.93	0.69
1:B:190:LEU:HD12	1:B:207:ILE:HG12	1.74	0.69
1:C:136:HIS:O	1:C:140:VAL:HG23	1.93	0.69
1:F:252:VAL:HG11	1:F:258:ILE:HD11	1.75	0.69
1:B:136:HIS:O	1:B:140:VAL:HG23	1.93	0.69
1:C:97:GLU:HG3	1:G:51:LEU:HD11	1.75	0.69
1:D:136:HIS:O	1:D:140:VAL:HG23	1.93	0.69
1:D:327:SER:HB2	1:D:459:ILE:HD11	1.75	0.69
1:F:406:PRO:HA	1:F:453:THR:HG22	1.75	0.69
1:G:4:GLU:O	1:G:8:ARG:HB2	1.93	0.69
1:C:64:GLN:HA	1:C:64:GLN:HE21	1.58	0.69
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.74	0.69
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.58	0.69
1:D:397:VAL:HG21	1:D:468:VAL:HG21	1.75	0.69
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.58	0.68
1:B:97:GLU:CG	1:I:51:LEU:HD13	2.15	0.68
1:D:233:ARG:HG3	1:D:233:ARG:HH11	1.58	0.68
1:E:136:HIS:O	1:E:140:VAL:HG23	1.93	0.68
1:C:463:PHE:O	1:C:467:VAL:HB	1.93	0.68
1:H:4:GLU:O	1:H:8:ARG:HB2	1.93	0.68
1:B:64:GLN:HA	1:B:64:GLN:HE21	1.58	0.68
1:D:302:LEU:HD23	1:D:337:PHE:CE1	2.29	0.68
1:A:212:LYS:HE3	1:A:238:ALA:HB1	1.75	0.68
1:F:136:HIS:O	1:F:140:VAL:HG23	1.93	0.68
1:A:136:HIS:O	1:A:140:VAL:HG23	1.93	0.68
1:A:302:LEU:HD23	1:A:337:PHE:CE1	2.29	0.68
1:C:395:PHE:HB3	1:C:413:VAL:CB	2.18	0.68
1:D:205:THR:HA	1:D:231:LEU:HD11	1.75	0.67
1:A:96:ASN:O	1:A:98:PRO:HD3	1.94	0.67
1:C:40:HIS:ND1	1:C:60:ILE:HD13	2.07	0.67
1:C:96:ASN:O	1:C:98:PRO:HD3	1.94	0.67
1:F:302:LEU:HD23	1:F:337:PHE:CE1	2.29	0.67
1:G:42:GLU:O	1:G:46:LYS:HG3	1.95	0.67
1:E:302:LEU:HD23	1:E:337:PHE:CE1	2.29	0.67
1:B:96:ASN:O	1:B:98:PRO:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:HA	1:A:484:LEU:HD22	1.77	0.67
1:B:393:LEU:HD21	1:B:464:LEU:HD22	1.76	0.67
1:C:302:LEU:HD23	1:C:337:PHE:CE1	2.29	0.67
1:A:64:GLN:HE21	1:A:64:GLN:HA	1.58	0.67
1:C:30:LEU:HD22	1:C:35:ILE:HD12	1.75	0.67
1:C:115:LEU:CD2	1:C:180:ILE:HB	2.25	0.67
1:D:456:ILE:HG13	1:D:460:ILE:HG23	1.77	0.67
1:F:388:GLU:HB3	1:F:433:ARG:HH21	1.58	0.67
1:B:115:LEU:CD2	1:B:180:ILE:HB	2.26	0.66
1:C:123:ASN:OD1	1:F:229:VAL:HG23	1.95	0.66
1:A:334:MET:HE1	1:A:337:PHE:HD2	1.60	0.66
1:D:314:LYS:O	1:D:318:VAL:HG23	1.96	0.66
1:C:208:LEU:HD23	1:C:235:ILE:HA	1.77	0.66
1:C:143:LYS:O	1:C:147:MET:HG3	1.96	0.66
1:D:143:LYS:O	1:D:147:MET:HG3	1.96	0.66
1:E:314:LYS:O	1:E:318:VAL:HG23	1.95	0.66
1:A:529:PHE:HB3	1:A:532:PHE:CE1	2.31	0.66
1:E:479:ILE:HG23	1:E:483:ARG:NH2	2.11	0.66
1:I:42:GLU:O	1:I:46:LYS:HG3	1.95	0.66
1:A:462:MET:HG2	1:A:465:LYS:HE3	1.78	0.66
1:B:123:ASN:OD1	1:D:229:VAL:CG2	2.44	0.66
1:C:212:LYS:HE3	1:C:238:ALA:HB1	1.77	0.66
1:D:115:LEU:CD2	1:D:180:ILE:HB	2.26	0.66
1:A:485:LEU:HD23	1:A:485:LEU:H	1.59	0.66
1:B:347:LYS:O	1:B:347:LYS:HD3	1.96	0.66
1:A:456:ILE:HG13	1:A:460:ILE:HG23	1.77	0.66
1:B:208:LEU:HB2	1:B:235:ILE:HG12	1.78	0.66
1:B:529:PHE:HB3	1:B:532:PHE:CE1	2.31	0.66
1:C:29:TYR:CZ	1:C:33:LYS:HD2	2.30	0.66
1:E:211:LEU:HD22	1:E:242:ARG:HG3	1.78	0.66
1:E:529:PHE:HB3	1:E:532:PHE:CE1	2.31	0.66
1:F:529:PHE:HB3	1:F:532:PHE:CE1	2.31	0.66
1:H:42:GLU:O	1:H:46:LYS:HG3	1.95	0.66
1:C:347:LYS:O	1:C:347:LYS:HD3	1.96	0.65
1:F:393:LEU:HD21	1:F:464:LEU:HD22	1.77	0.65
1:I:72:ILE:HG21	1:I:88:GLU:HG3	1.78	0.65
1:F:143:LYS:O	1:F:147:MET:HG3	1.96	0.65
1:F:334:MET:HE1	1:F:337:PHE:HD2	1.62	0.65
1:A:327:SER:HB2	1:A:459:ILE:HD11	1.76	0.65
1:C:97:GLU:OE2	1:G:51:LEU:CD1	2.13	0.65
1:F:115:LEU:CD2	1:F:180:ILE:HB	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:O	1:B:147:MET:HG3	1.96	0.65
1:A:393:LEU:HD23	1:A:464:LEU:HD11	1.78	0.65
1:B:456:ILE:HG13	1:B:460:ILE:HG23	1.78	0.65
1:D:347:LYS:O	1:D:347:LYS:HD3	1.96	0.65
1:D:529:PHE:HB3	1:D:532:PHE:CE1	2.31	0.65
1:F:158:HIS:NE2	1:F:287:PHE:HB3	2.12	0.65
1:G:37:THR:OG1	1:G:40:HIS:HD2	1.79	0.65
1:A:347:LYS:O	1:A:347:LYS:HD3	1.96	0.65
1:C:236:CYS:SG	1:E:121:LEU:HD23	2.37	0.65
1:A:143:LYS:O	1:A:147:MET:HG3	1.96	0.65
1:C:32:GLY:C	1:C:34:ASN:H	1.98	0.65
1:C:120:LEU:HD21	1:F:236:CYS:SG	2.35	0.65
1:E:143:LYS:O	1:E:147:MET:HG3	1.96	0.65
1:B:29:TYR:O	1:B:33:LYS:HG3	1.97	0.65
1:B:233:ARG:NH1	1:F:121:LEU:HD22	2.10	0.65
1:C:283:GLN:HG2	1:C:284:THR:H	1.60	0.65
1:H:72:ILE:HG21	1:H:88:GLU:HG3	1.78	0.65
1:D:485:LEU:HD23	1:D:485:LEU:H	1.62	0.65
1:E:112:ARG:NH1	1:E:115:LEU:HD12	2.12	0.65
1:F:112:ARG:NH1	1:F:115:LEU:HD12	2.12	0.65
1:F:231:LEU:O	1:F:235:ILE:HG13	1.96	0.65
1:F:437:LEU:HD12	1:F:444:LEU:HD22	1.79	0.65
1:G:77:TYR:CD1	1:G:77:TYR:C	2.71	0.64
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.79	0.64
1:D:112:ARG:NH1	1:D:115:LEU:HD12	2.12	0.64
1:E:115:LEU:CD2	1:E:180:ILE:HB	2.26	0.64
1:G:10:LEU:HD22	1:G:58:LEU:HD21	1.80	0.64
1:H:37:THR:OG1	1:H:40:HIS:HD2	1.79	0.64
1:C:464:LEU:O	1:C:468:VAL:HG22	1.98	0.64
1:I:10:LEU:HD22	1:I:58:LEU:HD21	1.80	0.64
1:I:37:THR:OG1	1:I:40:HIS:HD2	1.79	0.64
1:C:236:CYS:HB2	1:E:120:LEU:CD2	2.19	0.64
1:E:475:ASN:O	1:E:479:ILE:HG13	1.98	0.64
1:A:4:GLU:O	1:A:8:ARG:HB2	1.97	0.64
1:A:211:LEU:HD11	1:A:239:LEU:HD23	1.79	0.64
1:F:315:GLU:HA	1:F:318:VAL:HG23	1.80	0.64
1:F:347:LYS:O	1:F:347:LYS:HD3	1.96	0.64
1:F:475:ASN:O	1:F:479:ILE:HG13	1.98	0.64
1:H:77:TYR:C	1:H:77:TYR:CD1	2.71	0.64
1:B:534:GLN:HA	1:B:534:GLN:NE2	2.13	0.64
1:C:334:MET:HE1	1:C:337:PHE:HD2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LEU:CD2	1:D:460:ILE:HD11	2.27	0.64
1:A:315:GLU:HA	1:A:318:VAL:HG23	1.80	0.64
1:D:334:MET:HE1	1:D:337:PHE:HD2	1.63	0.64
1:E:159:GLY:N	1:E:165:LYS:HD3	2.13	0.64
1:F:141:ILE:HG23	1:F:179:LEU:CD2	2.28	0.64
1:I:77:TYR:CD1	1:I:77:TYR:C	2.71	0.64
1:A:141:ILE:HG23	1:A:179:LEU:CD2	2.29	0.63
1:D:475:ASN:O	1:D:479:ILE:HG13	1.98	0.63
1:A:534:GLN:HA	1:A:534:GLN:NE2	2.13	0.63
1:B:405:ILE:HG12	1:B:410:TRP:CZ3	2.34	0.63
1:C:141:ILE:HG23	1:C:179:LEU:CD2	2.29	0.63
1:A:106:ILE:CG2	1:A:182:ILE:HA	2.28	0.63
1:A:313:GLU:O	1:A:316:GLU:HG3	1.97	0.63
1:B:315:GLU:HA	1:B:318:VAL:HG23	1.80	0.63
1:D:141:ILE:HG23	1:D:179:LEU:CD2	2.29	0.63
1:E:405:ILE:HG12	1:E:410:TRP:CZ3	2.34	0.63
1:E:464:LEU:O	1:E:468:VAL:HG22	1.98	0.63
1:F:190:LEU:HD12	1:F:207:ILE:HG12	1.79	0.63
1:F:310:PRO:HA	1:F:345:PHE:HZ	1.61	0.63
1:B:205:THR:HA	1:B:231:LEU:HD11	1.80	0.63
1:D:239:LEU:HD22	1:D:242:ARG:HB2	1.80	0.63
1:E:141:ILE:HG23	1:E:179:LEU:CD2	2.29	0.63
1:F:405:ILE:HG12	1:F:410:TRP:CZ3	2.34	0.63
1:B:8:ARG:HG2	1:B:8:ARG:NH1	2.10	0.63
1:C:534:GLN:HA	1:C:534:GLN:NE2	2.13	0.63
1:D:405:ILE:HG12	1:D:410:TRP:CZ3	2.34	0.63
1:F:184:TYR:HA	1:F:244:ASN:HB3	1.80	0.63
1:A:443:LEU:CD2	1:A:460:ILE:HD11	2.27	0.63
1:A:475:ASN:O	1:A:479:ILE:HG13	1.98	0.63
1:A:478:SER:O	1:A:482:GLN:HG2	1.98	0.63
1:C:529:PHE:HB3	1:C:532:PHE:CZ	2.34	0.63
1:E:334:MET:HE1	1:E:337:PHE:HD2	1.64	0.63
1:C:115:LEU:HD11	1:C:177:ASP:HA	1.81	0.63
1:A:8:ARG:NE	1:A:244:ASN:HD22	1.96	0.63
1:B:236:CYS:CB	1:F:120:LEU:HD21	2.20	0.63
1:C:315:GLU:HA	1:C:318:VAL:HG23	1.80	0.63
1:C:405:ILE:HG12	1:C:410:TRP:CZ3	2.34	0.63
1:A:405:ILE:HG12	1:A:410:TRP:CZ3	2.34	0.63
1:C:475:ASN:O	1:C:479:ILE:HG13	1.98	0.62
1:C:126:LYS:HG3	1:F:265:ARG:HH21	1.64	0.62
1:E:534:GLN:HA	1:E:534:GLN:NE2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:534:GLN:HA	1:F:534:GLN:NE2	2.13	0.62
1:D:534:GLN:HA	1:D:534:GLN:NE2	2.13	0.62
1:G:17:LEU:HD23	1:G:21:PHE:CD2	2.35	0.62
1:H:10:LEU:HD22	1:H:58:LEU:HD21	1.80	0.62
1:H:47:MET:HB2	1:H:53:ARG:CG	2.29	0.62
1:A:75:PHE:CB	1:A:84:ALA:HB2	2.29	0.62
1:B:141:ILE:HG23	1:B:179:LEU:CD2	2.29	0.62
1:G:10:LEU:HD13	1:G:58:LEU:CD2	2.29	0.62
1:B:8:ARG:HH11	1:B:8:ARG:CG	2.12	0.62
1:C:35:ILE:HD11	1:C:70:PRO:HG2	1.81	0.62
1:A:122:GLY:HA3	1:A:187:ILE:HG23	1.82	0.62
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.35	0.62
1:C:42:GLU:O	1:C:46:LYS:HG3	2.00	0.62
1:C:72:ILE:HD11	1:C:87:LEU:HB2	1.81	0.62
1:H:17:LEU:HD23	1:H:21:PHE:CD2	2.35	0.62
1:B:121:LEU:CD2	1:D:233:ARG:NE	2.60	0.62
1:A:42:GLU:O	1:A:46:LYS:HG3	2.00	0.62
1:H:10:LEU:HD13	1:H:58:LEU:CD2	2.30	0.62
1:C:190:LEU:CD1	1:C:207:ILE:HG12	2.30	0.61
1:F:122:GLY:HA3	1:F:187:ILE:HG23	1.82	0.61
1:F:189:TRP:CE3	1:F:248:VAL:HG11	2.35	0.61
1:G:8:ARG:HG2	1:G:8:ARG:NH1	2.11	0.61
1:C:90:TYR:CE2	1:C:106:ILE:HD11	2.28	0.61
1:D:189:TRP:CE3	1:D:248:VAL:HG11	2.35	0.61
1:G:47:MET:HB2	1:G:53:ARG:CG	2.29	0.61
1:B:77:TYR:CD1	1:B:77:TYR:C	2.73	0.61
1:C:453:THR:HG21	1:C:524:ILE:CD1	2.30	0.61
1:D:122:GLY:HA3	1:D:187:ILE:HG23	1.82	0.61
1:A:309:MET:HG3	1:A:310:PRO:HD2	1.81	0.61
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.35	0.61
1:B:532:PHE:C	1:B:534:GLN:H	2.04	0.61
1:I:10:LEU:HD13	1:I:58:LEU:CD2	2.29	0.61
1:A:47:MET:HB2	1:A:53:ARG:CG	2.30	0.61
1:C:77:TYR:C	1:C:77:TYR:CD1	2.73	0.61
1:C:265:ARG:HH21	1:E:125:PRO:C	2.04	0.61
1:E:189:TRP:CE3	1:E:248:VAL:HG11	2.35	0.61
1:C:189:TRP:CE3	1:C:248:VAL:HG11	2.35	0.61
1:E:532:PHE:C	1:E:534:GLN:H	2.04	0.61
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.30	0.61
1:D:388:GLU:HB3	1:D:433:ARG:HH21	1.66	0.61
1:F:159:GLY:N	1:F:165:LYS:HD3	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:MET:HB2	1:C:53:ARG:CG	2.30	0.61
1:I:17:LEU:HD23	1:I:21:PHE:CD2	2.35	0.61
1:D:532:PHE:C	1:D:534:GLN:H	2.04	0.61
1:E:122:GLY:HA3	1:E:187:ILE:HG23	1.82	0.61
1:A:8:ARG:HH11	1:A:8:ARG:CG	2.12	0.61
1:A:37:THR:H	1:A:40:HIS:HB2	1.66	0.61
1:C:388:GLU:HB3	1:C:433:ARG:HH21	1.66	0.61
1:F:133:ARG:O	1:F:137:VAL:HG23	2.01	0.61
1:E:457:ASP:O	1:E:461:HIS:HB2	1.99	0.60
1:F:136:HIS:HB3	1:F:168:ILE:HD13	1.83	0.60
1:H:8:ARG:HG2	1:H:8:ARG:NH1	2.11	0.60
1:B:208:LEU:HD23	1:B:235:ILE:CA	2.23	0.60
1:F:313:GLU:O	1:F:316:GLU:HG3	2.00	0.60
1:H:37:THR:OG1	1:H:40:HIS:CD2	2.54	0.60
1:I:37:THR:OG1	1:I:40:HIS:CD2	2.54	0.60
1:B:17:LEU:HD23	1:B:21:PHE:CD2	2.37	0.60
1:B:42:GLU:O	1:B:46:LYS:HG3	2.00	0.60
1:B:122:GLY:HA3	1:B:187:ILE:HG23	1.82	0.60
1:C:407:VAL:HG23	1:C:452:LEU:O	2.02	0.60
1:D:407:VAL:HG23	1:D:452:LEU:O	2.02	0.60
1:G:37:THR:OG1	1:G:40:HIS:CD2	2.54	0.60
1:I:47:MET:HB2	1:I:53:ARG:CG	2.29	0.60
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.66	0.60
1:B:525:ARG:NE	1:B:525:ARG:H	2.00	0.60
1:E:388:GLU:HB3	1:E:433:ARG:HH21	1.66	0.60
1:F:532:PHE:C	1:F:534:GLN:H	2.04	0.60
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.37	0.60
1:A:388:GLU:HB3	1:A:433:ARG:HH21	1.66	0.60
1:C:122:GLY:HA3	1:C:187:ILE:HG23	1.82	0.60
1:C:133:ARG:O	1:C:137:VAL:HG23	2.01	0.60
1:D:136:HIS:HB3	1:D:168:ILE:HD13	1.83	0.60
1:E:309:MET:N	1:E:309:MET:SD	2.75	0.60
1:B:121:LEU:CB	1:D:233:ARG:HE	2.14	0.60
1:B:407:VAL:HG23	1:B:452:LEU:O	2.02	0.60
1:C:10:LEU:HD22	1:C:58:LEU:HD21	1.84	0.60
1:E:407:VAL:HG23	1:E:452:LEU:O	2.02	0.60
1:F:437:LEU:HB3	1:F:444:LEU:HD22	1.82	0.60
1:B:133:ARG:O	1:B:137:VAL:HG23	2.01	0.60
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.82	0.60
1:D:133:ARG:O	1:D:137:VAL:HG23	2.01	0.60
1:A:136:HIS:HB3	1:A:168:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ILE:O	1:F:483:ARG:HD3	2.01	0.60
1:F:283:GLN:HG2	1:F:284:THR:H	1.67	0.60
1:A:10:LEU:HD22	1:A:58:LEU:HD21	1.84	0.59
1:B:10:LEU:HD22	1:B:58:LEU:HD21	1.84	0.59
1:A:532:PHE:C	1:A:534:GLN:H	2.04	0.59
1:B:47:MET:HB2	1:B:53:ARG:CG	2.30	0.59
1:E:255:GLU:HA	1:E:258:ILE:HD13	1.84	0.59
1:A:127:GLN:HB2	1:A:171:GLN:CG	2.31	0.59
1:C:136:HIS:HB3	1:C:168:ILE:HD13	1.83	0.59
1:D:159:GLY:N	1:D:165:LYS:HD3	2.17	0.59
1:B:240:ILE:HG22	1:F:117:ARG:NH1	2.11	0.59
1:A:407:VAL:HG23	1:A:452:LEU:O	2.02	0.59
1:B:525:ARG:H	1:B:525:ARG:HE	1.51	0.59
1:C:532:PHE:C	1:C:534:GLN:H	2.04	0.59
1:A:112:ARG:HA	1:A:115:LEU:HG	1.85	0.59
1:G:50:ARG:HA	1:G:53:ARG:HE	1.68	0.59
1:B:10:LEU:HD13	1:B:58:LEU:CD2	2.33	0.59
1:C:17:LEU:HD23	1:C:21:PHE:CD2	2.37	0.59
1:C:258:ILE:HD12	1:C:258:ILE:H	1.66	0.59
1:D:368:PRO:HB2	3:D:602:ATP:O3'	2.03	0.59
1:E:133:ARG:O	1:E:137:VAL:HG23	2.01	0.59
1:A:74:PHE:HD2	1:A:77:TYR:HE2	1.51	0.59
1:E:128:MET:HB2	1:E:171:GLN:HE21	1.68	0.59
1:E:136:HIS:HB3	1:E:168:ILE:HD13	1.83	0.59
1:F:407:VAL:HG23	1:F:452:LEU:O	2.02	0.59
1:A:50:ARG:HA	1:A:53:ARG:HE	1.68	0.59
1:A:133:ARG:O	1:A:137:VAL:HG23	2.01	0.59
1:D:255:GLU:HA	1:D:258:ILE:HD13	1.85	0.59
3:F:602:ATP:O1B	3:F:602:ATP:O2G	2.21	0.59
1:B:368:PRO:HB2	3:B:602:ATP:O3'	2.03	0.58
1:F:368:PRO:HB2	3:F:602:ATP:O3'	2.03	0.58
1:C:368:PRO:HB2	3:C:602:ATP:O3'	2.03	0.58
1:I:8:ARG:HG2	1:I:8:ARG:NH1	2.11	0.58
1:A:10:LEU:HD13	1:A:58:LEU:CD2	2.33	0.58
1:C:50:ARG:HA	1:C:53:ARG:HE	1.68	0.58
1:C:112:ARG:NH1	1:C:115:LEU:HD12	2.18	0.58
1:C:120:LEU:CD2	1:F:236:CYS:HB2	2.19	0.58
1:D:262:GLN:NE2	1:D:283:GLN:HB2	2.18	0.58
1:E:368:PRO:HB2	3:E:602:ATP:O3'	2.03	0.58
1:I:50:ARG:HA	1:I:53:ARG:HE	1.68	0.58
3:A:602:ATP:O1B	3:A:602:ATP:O2G	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:LEU:HD13	1:C:58:LEU:CD2	2.33	0.58
1:H:50:ARG:HA	1:H:53:ARG:HE	1.68	0.58
1:I:23:PRO:HG2	1:I:53:ARG:C	2.24	0.58
1:D:190:LEU:HD12	1:D:207:ILE:HG12	1.84	0.58
1:D:447:LYS:HE2	1:D:450:PRO:HD2	1.85	0.58
1:A:237:ASN:O	1:A:240:ILE:HG23	2.03	0.58
1:B:136:HIS:HB3	1:B:168:ILE:HD13	1.83	0.58
1:H:23:PRO:HG2	1:H:53:ARG:C	2.24	0.58
1:F:521:GLU:C	1:F:523:VAL:H	2.07	0.58
1:C:68:LEU:O	1:C:68:LEU:HD13	2.04	0.58
1:C:29:TYR:CE2	1:C:33:LYS:HD2	2.39	0.58
1:B:25:ASP:HB3	1:B:78:ASN:HD21	1.69	0.58
1:D:248:VAL:HG22	1:D:269:LEU:HB3	1.86	0.58
1:D:521:GLU:C	1:D:523:VAL:H	2.07	0.58
1:F:248:VAL:HG22	1:F:269:LEU:HB3	1.86	0.58
1:B:258:ILE:H	1:B:258:ILE:HD12	1.69	0.57
1:B:393:LEU:HD23	1:B:394:ALA:N	2.19	0.57
1:D:527:GLU:HA	1:D:530:PRO:HG3	1.86	0.57
1:A:101:LEU:HD12	1:A:105:VAL:HB	1.86	0.57
3:B:602:ATP:O1B	3:B:602:ATP:O2G	2.21	0.57
1:C:248:VAL:HG22	1:C:269:LEU:HB3	1.86	0.57
1:C:526:PRO:HB2	1:C:529:PHE:HB2	1.86	0.57
1:E:205:THR:HA	1:E:231:LEU:HD11	1.86	0.57
1:E:347:LYS:NZ	1:E:351:LEU:HD21	2.20	0.57
3:E:602:ATP:O1B	3:E:602:ATP:O2G	2.21	0.57
1:F:253:VAL:HG11	1:F:380:ARG:HD3	1.86	0.57
1:F:309:MET:HG3	1:F:310:PRO:HD2	1.85	0.57
1:F:456:ILE:HD11	1:F:461:HIS:HA	1.86	0.57
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.86	0.57
1:A:368:PRO:HB2	3:A:602:ATP:O3'	2.03	0.57
1:A:542:SER:O	1:A:543:LEU:HD22	2.05	0.57
1:B:68:LEU:O	1:B:68:LEU:HD13	2.04	0.57
1:C:542:SER:O	1:C:543:LEU:HD22	2.05	0.57
1:A:310:PRO:HA	1:A:345:PHE:CZ	2.40	0.57
1:C:23:PRO:HG2	1:C:53:ARG:C	2.24	0.57
3:D:602:ATP:O1B	3:D:602:ATP:O2G	2.21	0.57
1:A:527:GLU:HA	1:A:530:PRO:HG3	1.86	0.57
1:I:49:THR:HG22	1:I:50:ARG:N	2.20	0.57
1:B:1:MET:CE	1:F:117:ARG:CZ	2.83	0.57
1:B:233:ARG:CZ	1:F:121:LEU:HD22	2.35	0.57
3:C:602:ATP:O1B	3:C:602:ATP:O2G	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:SER:O	1:E:482:GLN:HG2	2.04	0.57
1:G:23:PRO:HG2	1:G:53:ARG:C	2.24	0.57
1:A:68:LEU:HD13	1:A:68:LEU:O	2.04	0.57
1:B:120:LEU:HD21	1:D:236:CYS:HB2	1.86	0.57
1:E:248:VAL:HG22	1:E:269:LEU:HB3	1.86	0.57
1:E:447:LYS:HE2	1:E:450:PRO:HD2	1.87	0.57
1:F:542:SER:O	1:F:543:LEU:HD22	2.04	0.57
1:I:68:LEU:HD13	1:I:68:LEU:O	2.05	0.57
1:B:50:ARG:HA	1:B:53:ARG:HE	1.68	0.57
1:D:253:VAL:HG11	1:D:380:ARG:NH1	2.20	0.57
1:A:23:PRO:HG2	1:A:53:ARG:C	2.24	0.57
1:F:527:GLU:HA	1:F:530:PRO:HG3	1.86	0.57
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.69	0.57
1:A:207:ILE:O	1:A:210:MET:N	2.38	0.57
1:B:23:PRO:HG2	1:B:53:ARG:C	2.24	0.57
1:B:542:SER:O	1:B:543:LEU:HD22	2.05	0.57
1:E:521:GLU:C	1:E:523:VAL:H	2.07	0.57
1:A:18:ILE:O	1:A:50:ARG:NH2	2.37	0.56
1:A:97:GLU:OE1	1:H:51:LEU:CB	2.50	0.56
1:A:253:VAL:HG11	1:A:380:ARG:HD3	1.86	0.56
1:A:521:GLU:C	1:A:523:VAL:H	2.08	0.56
1:G:68:LEU:O	1:G:68:LEU:HD13	2.05	0.56
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.86	0.56
1:E:542:SER:O	1:E:543:LEU:HD22	2.05	0.56
1:H:49:THR:HG22	1:H:50:ARG:N	2.20	0.56
1:B:214:GLU:OE2	1:D:233:ARG:NH2	2.35	0.56
1:B:334:MET:HE1	1:B:337:PHE:HD2	1.70	0.56
1:C:25:ASP:HB3	1:C:78:ASN:HD21	1.69	0.56
1:C:240:ILE:HG13	1:C:241:ASP:N	2.21	0.56
1:B:527:GLU:HA	1:B:530:PRO:HG3	1.87	0.56
1:G:18:ILE:O	1:G:50:ARG:NH2	2.37	0.56
1:A:464:LEU:O	1:A:468:VAL:HG22	2.06	0.56
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.88	0.56
1:B:248:VAL:HG22	1:B:269:LEU:HB3	1.86	0.56
1:D:208:LEU:HB2	1:D:235:ILE:HG12	1.87	0.56
1:G:49:THR:HG22	1:G:50:ARG:N	2.20	0.56
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.18	0.56
1:A:534:GLN:HE21	1:A:534:GLN:CA	2.18	0.56
1:D:258:ILE:H	1:D:258:ILE:HD12	1.70	0.56
1:D:542:SER:O	1:D:543:LEU:HD22	2.05	0.56
1:E:141:ILE:HD13	1:E:176:SER:CB	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:VAL:HG11	1:E:380:ARG:NH1	2.20	0.56
1:E:445:SER:HB3	1:E:455:LYS:HB3	1.86	0.56
1:B:205:THR:O	1:B:209:LEU:HG	2.06	0.56
1:C:93:PHE:HD2	1:C:100:LEU:HB3	1.70	0.56
1:C:253:VAL:HG11	1:C:380:ARG:HD3	1.86	0.56
1:F:237:ASN:O	1:F:240:ILE:HG23	2.06	0.56
1:F:403:VAL:HG12	1:F:405:ILE:HG22	1.88	0.56
1:H:25:ASP:HB3	1:H:78:ASN:HD21	1.70	0.56
1:C:32:GLY:C	1:C:34:ASN:N	2.59	0.55
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.18	0.55
1:D:534:GLN:HE21	1:D:534:GLN:CA	2.19	0.55
1:H:68:LEU:O	1:H:68:LEU:HD13	2.05	0.55
1:D:233:ARG:HH11	1:D:233:ARG:CG	2.17	0.55
1:D:403:VAL:HG12	1:D:405:ILE:HG22	1.89	0.55
1:I:18:ILE:O	1:I:50:ARG:NH2	2.37	0.55
1:B:527:GLU:C	1:B:530:PRO:HD3	2.27	0.55
1:B:93:PHE:HD2	1:B:100:LEU:HB3	1.70	0.55
1:D:341:GLU:HB3	1:D:342:PRO:HD3	1.89	0.55
1:E:527:GLU:HA	1:E:530:PRO:HG3	1.86	0.55
1:A:182:ILE:HD12	1:A:182:ILE:N	2.22	0.55
1:B:23:PRO:HG2	1:B:53:ARG:HB3	1.89	0.55
1:B:403:VAL:HG12	1:B:405:ILE:HG22	1.89	0.55
1:C:97:GLU:CG	1:G:51:LEU:HD13	2.19	0.55
1:D:329:ASN:HB2	1:D:459:ILE:HD13	1.88	0.55
1:E:258:ILE:H	1:E:258:ILE:HD12	1.72	0.55
1:F:141:ILE:HD12	1:F:175:LYS:HZ2	1.70	0.55
1:C:117:ARG:NH2	1:F:240:ILE:CB	2.68	0.55
1:D:157:LEU:HD11	1:D:168:ILE:CG2	2.37	0.55
1:A:93:PHE:HD2	1:A:100:LEU:HB3	1.70	0.55
1:B:97:GLU:OE2	1:I:51:LEU:CD1	2.22	0.55
1:B:117:ARG:NH1	1:D:240:ILE:HG22	2.17	0.55
1:B:182:ILE:N	1:B:182:ILE:HD12	2.22	0.55
1:D:182:ILE:N	1:D:182:ILE:HD12	2.22	0.55
1:E:479:ILE:HG23	1:E:483:ARG:HH22	1.68	0.55
1:F:240:ILE:HG13	1:F:241:ASP:N	2.21	0.55
1:I:25:ASP:HB3	1:I:78:ASN:HD21	1.70	0.55
1:B:332:THR:HG23	1:B:374:LEU:HB2	1.89	0.55
1:E:182:ILE:HD12	1:E:182:ILE:N	2.22	0.55
1:H:18:ILE:O	1:H:50:ARG:NH2	2.37	0.55
1:A:23:PRO:HG2	1:A:53:ARG:HB3	1.89	0.55
1:A:165:LYS:NZ	3:A:602:ATP:O1G	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:LEU:HD11	1:E:168:ILE:CG2	2.37	0.55
1:F:527:GLU:C	1:F:530:PRO:HD3	2.27	0.55
1:A:128:MET:HB2	1:A:171:GLN:NE2	2.22	0.55
1:A:527:GLU:C	1:A:530:PRO:HD3	2.27	0.55
1:D:165:LYS:NZ	3:D:602:ATP:O1G	2.40	0.55
1:D:354:LYS:HD3	1:D:362:GLY:O	2.07	0.55
1:A:98:PRO:O	1:A:99:ASP:HB2	2.06	0.54
1:B:112:ARG:NH1	1:B:115:LEU:HD12	2.22	0.54
1:C:23:PRO:HG2	1:C:53:ARG:HB3	1.89	0.54
1:C:161:ALA:HA	1:C:273:ARG:HD3	1.89	0.54
1:C:204:PHE:HA	1:C:207:ILE:HG13	1.87	0.54
1:E:332:THR:HG23	1:E:374:LEU:HB2	1.89	0.54
1:E:354:LYS:HD3	1:E:362:GLY:O	2.07	0.54
1:A:403:VAL:HG12	1:A:405:ILE:HG22	1.88	0.54
1:B:98:PRO:O	1:B:99:ASP:HB2	2.06	0.54
1:D:332:THR:HG23	1:D:374:LEU:HB2	1.89	0.54
1:E:211:LEU:HD11	1:E:235:ILE:HG23	1.89	0.54
1:G:77:TYR:O	1:G:77:TYR:HD1	1.90	0.54
1:A:385:LEU:CD1	1:A:393:LEU:HD12	2.37	0.54
1:B:354:LYS:HD3	1:B:362:GLY:O	2.07	0.54
1:C:157:LEU:HD11	1:C:168:ILE:CG2	2.37	0.54
1:C:354:LYS:HD3	1:C:362:GLY:O	2.07	0.54
1:D:527:GLU:C	1:D:530:PRO:HD3	2.27	0.54
1:E:165:LYS:NZ	3:E:602:ATP:O1G	2.40	0.54
1:E:403:VAL:HG12	1:E:405:ILE:HG22	1.88	0.54
1:F:182:ILE:HD12	1:F:182:ILE:N	2.22	0.54
1:G:25:ASP:HB3	1:G:78:ASN:HD21	1.71	0.54
1:A:354:LYS:HD3	1:A:362:GLY:O	2.07	0.54
1:C:434:LEU:HD22	1:C:444:LEU:HD22	1.88	0.54
1:F:157:LEU:HD11	1:F:168:ILE:CG2	2.37	0.54
1:F:332:THR:HG23	1:F:374:LEU:HB2	1.89	0.54
1:A:157:LEU:HD11	1:A:168:ILE:CG2	2.37	0.54
1:C:212:LYS:HE3	1:C:238:ALA:CB	2.37	0.54
1:E:527:GLU:C	1:E:530:PRO:HD3	2.27	0.54
1:G:29:TYR:CZ	1:G:33:LYS:HD2	2.43	0.54
1:H:29:TYR:CZ	1:H:33:LYS:HD2	2.43	0.54
1:A:177:ASP:O	1:A:182:ILE:HD13	2.08	0.54
1:B:157:LEU:HD11	1:B:168:ILE:CG2	2.37	0.54
1:D:252:VAL:HG11	1:D:258:ILE:HD11	1.90	0.54
1:D:385:LEU:CD1	1:D:393:LEU:HD12	2.37	0.54
1:E:208:LEU:HD21	1:E:234:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:NZ	3:F:602:ATP:O1G	2.40	0.54
1:I:77:TYR:HD1	1:I:77:TYR:O	1.90	0.54
1:A:141:ILE:HD12	1:A:175:LYS:NZ	2.23	0.54
1:C:101:LEU:HD12	1:C:105:VAL:HB	1.90	0.54
1:C:182:ILE:HD12	1:C:182:ILE:N	2.22	0.54
1:D:214:GLU:CD	1:D:214:GLU:H	2.11	0.54
1:E:211:LEU:HA	1:E:242:ARG:HH21	1.72	0.54
1:F:354:LYS:HD3	1:F:362:GLY:O	2.07	0.54
1:H:77:TYR:O	1:H:77:TYR:HD1	1.90	0.54
1:E:239:LEU:HD13	1:E:242:ARG:HB2	1.89	0.54
1:C:77:TYR:O	1:C:77:TYR:HD1	1.91	0.54
1:E:208:LEU:HD23	1:E:235:ILE:HA	1.89	0.54
1:I:29:TYR:CZ	1:I:33:LYS:HD2	2.43	0.54
1:B:524:ILE:HD12	1:B:525:ARG:HE	1.73	0.53
1:C:18:ILE:O	1:C:50:ARG:NH2	2.37	0.53
1:C:105:VAL:O	1:C:105:VAL:HG12	2.08	0.53
1:D:344:THR:HG22	1:D:346:GLU:H	1.72	0.53
1:E:460:ILE:O	1:E:464:LEU:HG	2.08	0.53
1:A:160:ARG:HG2	1:A:442:ALA:HB3	1.90	0.53
1:C:98:PRO:O	1:C:99:ASP:HB2	2.06	0.53
1:C:403:VAL:HG12	1:C:405:ILE:HG22	1.88	0.53
1:H:9:ALA:HB2	1:H:90:TYR:CE1	2.44	0.53
1:B:4:GLU:HG3	1:B:5:ILE:N	2.24	0.53
1:G:10:LEU:HD13	1:G:58:LEU:HD22	1.90	0.53
1:A:332:THR:HG23	1:A:374:LEU:HB2	1.89	0.53
1:B:443:LEU:HA	1:B:460:ILE:HG12	1.91	0.53
1:C:9:ALA:HB2	1:C:90:TYR:CE1	2.44	0.53
1:C:324:GLU:HG3	1:C:458:HIS:CE1	2.44	0.53
1:I:26:ALA:HA	1:I:74:PHE:CE2	2.44	0.53
1:B:219:ASN:O	1:B:220:PHE:C	2.47	0.53
1:D:434:LEU:HD22	1:D:444:LEU:HD22	1.89	0.53
1:F:127:GLN:HB2	1:F:171:GLN:HG2	1.91	0.53
1:F:219:ASN:O	1:F:220:PHE:C	2.47	0.53
1:B:9:ALA:HB2	1:B:90:TYR:CE1	2.44	0.53
1:E:310:PRO:HB3	1:E:316:GLU:CA	2.38	0.53
1:F:484:LEU:HD11	1:F:533:MET:H	1.73	0.53
1:A:479:ILE:O	1:A:483:ARG:HD3	2.09	0.53
1:H:10:LEU:HD13	1:H:58:LEU:HD22	1.90	0.53
1:I:9:ALA:HB2	1:I:90:TYR:CE1	2.44	0.53
1:A:115:LEU:HD11	1:A:177:ASP:HA	1.90	0.53
1:A:159:GLY:H	1:A:165:LYS:HD3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:O	1:B:105:VAL:HG12	2.08	0.53
1:B:106:ILE:CG2	1:B:182:ILE:HA	2.39	0.53
1:C:72:ILE:CD1	1:C:87:LEU:HB2	2.39	0.53
1:C:240:ILE:HG13	1:C:241:ASP:OD1	2.08	0.53
1:F:240:ILE:HG13	1:F:241:ASP:OD1	2.08	0.53
1:C:534:GLN:HE21	1:C:534:GLN:CA	2.19	0.53
1:A:9:ALA:HB2	1:A:90:TYR:CE1	2.44	0.52
1:B:121:LEU:HD22	1:D:233:ARG:CZ	2.38	0.52
1:C:453:THR:HG21	1:C:524:ILE:HD11	1.91	0.52
1:A:185:ASP:H	1:A:244:ASN:HB3	1.73	0.52
1:C:8:ARG:HG2	1:C:8:ARG:NH1	2.10	0.52
1:C:332:THR:HG23	1:C:374:LEU:HB2	1.89	0.52
1:D:219:ASN:O	1:D:220:PHE:C	2.47	0.52
1:E:236:CYS:HA	1:E:239:LEU:HB2	1.91	0.52
1:E:274:ASP:C	1:E:274:ASP:OD1	2.48	0.52
1:A:8:ARG:HG2	1:A:8:ARG:NH1	2.10	0.52
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.91	0.52
1:A:437:LEU:HD12	1:A:444:LEU:HD23	1.91	0.52
1:B:101:LEU:HD12	1:B:105:VAL:HB	1.90	0.52
1:F:391:SER:O	1:F:395:PHE:HD2	1.91	0.52
1:I:10:LEU:HD13	1:I:58:LEU:HD22	1.90	0.52
1:A:219:ASN:O	1:A:220:PHE:C	2.47	0.52
1:A:234:MET:CE	1:D:217:LEU:HD12	2.40	0.52
1:A:274:ASP:C	1:A:274:ASP:OD1	2.48	0.52
1:B:159:GLY:N	1:B:165:LYS:HD3	2.25	0.52
1:E:310:PRO:HB3	1:E:316:GLU:HA	1.90	0.52
1:F:112:ARG:HH11	1:F:115:LEU:HD12	1.75	0.52
1:F:255:GLU:O	1:F:259:ARG:HG3	2.09	0.52
1:D:231:LEU:O	1:D:235:ILE:HG13	2.09	0.52
1:E:112:ARG:HH11	1:E:115:LEU:HD12	1.75	0.52
1:E:231:LEU:O	1:E:235:ILE:HG13	2.09	0.52
1:E:255:GLU:O	1:E:259:ARG:HG3	2.10	0.52
1:F:157:LEU:HD11	1:F:168:ILE:HG22	1.92	0.52
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.10	0.52
1:B:269:LEU:HD22	1:B:270:VAL:H	1.75	0.52
1:C:157:LEU:HD11	1:C:168:ILE:HG22	1.92	0.52
1:D:483:ARG:N	1:D:483:ARG:HD2	2.25	0.52
1:E:219:ASN:O	1:E:220:PHE:C	2.47	0.52
1:F:205:THR:O	1:F:209:LEU:HG	2.10	0.52
1:G:9:ALA:HB2	1:G:90:TYR:CE1	2.44	0.52
1:C:142:LYS:HE2	1:C:146:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ILE:HG21	1:G:88:GLU:HG3	1.92	0.52
1:A:233:ARG:NH1	1:A:237:ASN:HD21	2.07	0.52
1:B:21:PHE:CD1	1:B:75:PHE:HE1	2.27	0.52
1:C:242:ARG:HB3	1:C:245:THR:OG1	2.09	0.52
1:D:142:LYS:HE2	1:D:146:GLU:OE2	2.10	0.52
1:D:157:LEU:HD11	1:D:168:ILE:HG22	1.92	0.52
1:D:327:SER:HB2	1:D:459:ILE:CG1	2.40	0.52
1:D:484:LEU:HD13	1:D:533:MET:HG2	1.91	0.52
1:E:128:MET:HE2	1:E:128:MET:HA	1.90	0.52
1:E:534:GLN:HE21	1:E:534:GLN:CA	2.18	0.52
1:F:208:LEU:O	1:F:212:LYS:HG2	2.09	0.52
1:B:106:ILE:HG21	1:B:182:ILE:HA	1.92	0.52
1:B:211:LEU:HA	1:B:242:ARG:CZ	2.39	0.52
1:B:344:THR:HG22	1:B:346:GLU:H	1.75	0.52
1:B:529:PHE:N	1:B:530:PRO:CD	2.73	0.52
1:F:115:LEU:HD11	1:F:177:ASP:HA	1.92	0.52
1:F:342:PRO:C	1:F:344:THR:H	2.12	0.52
1:H:26:ALA:HA	1:H:74:PHE:CE2	2.44	0.52
1:A:283:GLN:HG3	1:D:126:LYS:HZ2	1.75	0.52
1:B:327:SER:HB2	1:B:459:ILE:CD1	2.39	0.52
1:E:157:LEU:HD23	1:E:288:ILE:HB	1.90	0.52
1:E:529:PHE:N	1:E:530:PRO:CD	2.73	0.52
1:B:77:TYR:O	1:B:77:TYR:HD1	1.91	0.51
1:C:21:PHE:CD1	1:C:75:PHE:HE1	2.27	0.51
1:C:274:ASP:C	1:C:274:ASP:OD1	2.48	0.51
1:D:112:ARG:HH11	1:D:115:LEU:HD12	1.75	0.51
1:F:212:LYS:HE2	1:F:212:LYS:HA	1.91	0.51
1:F:478:SER:O	1:F:482:GLN:HG2	2.10	0.51
1:H:23:PRO:HG2	1:H:53:ARG:HB3	1.92	0.51
1:A:529:PHE:N	1:A:530:PRO:CD	2.73	0.51
1:B:142:LYS:HE2	1:B:146:GLU:OE2	2.10	0.51
1:B:231:LEU:O	1:B:235:ILE:HG13	2.10	0.51
1:C:155:LEU:HD23	1:C:286:GLU:HB2	1.91	0.51
1:C:158:HIS:NE2	1:C:287:PHE:HB3	2.26	0.51
1:C:205:THR:O	1:C:209:LEU:HG	2.10	0.51
1:C:434:LEU:HB3	1:C:444:LEU:HD23	1.91	0.51
1:D:269:LEU:HD22	1:D:270:VAL:H	1.75	0.51
1:D:443:LEU:HA	1:D:460:ILE:HG12	1.93	0.51
1:F:444:LEU:O	1:F:445:SER:HB2	2.10	0.51
1:A:269:LEU:HD22	1:A:270:VAL:H	1.75	0.51
1:B:3:CYS:SG	1:B:5:ILE:HB	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASP:C	1:B:274:ASP:OD1	2.48	0.51
1:F:400:PRO:HD3	1:F:540:TYR:HE1	1.75	0.51
1:B:211:LEU:HA	1:B:242:ARG:NH1	2.25	0.51
1:I:21:PHE:CD1	1:I:75:PHE:HE1	2.29	0.51
1:A:484:LEU:O	1:A:531:LYS:HA	2.10	0.51
1:A:485:LEU:HG	1:A:486:GLU:H	1.76	0.51
1:B:35:ILE:HD11	1:B:70:PRO:HG2	1.93	0.51
1:C:219:ASN:O	1:C:220:PHE:C	2.47	0.51
1:C:231:LEU:O	1:C:235:ILE:HG13	2.11	0.51
1:D:529:PHE:N	1:D:530:PRO:CD	2.73	0.51
1:F:385:LEU:HB3	1:F:390:ARG:HG3	1.91	0.51
1:H:21:PHE:CD1	1:H:75:PHE:HE1	2.29	0.51
1:A:141:ILE:HG23	1:A:179:LEU:HD22	1.93	0.51
1:B:18:ILE:O	1:B:50:ARG:NH2	2.38	0.51
1:B:534:GLN:HE21	1:B:534:GLN:CA	2.18	0.51
1:E:142:LYS:HE2	1:E:146:GLU:OE2	2.10	0.51
1:F:258:ILE:H	1:F:258:ILE:HD12	1.75	0.51
1:A:74:PHE:HA	1:A:77:TYR:HD2	1.75	0.51
1:B:157:LEU:HD11	1:B:168:ILE:HG22	1.92	0.51
1:C:318:VAL:HG13	1:C:349:ALA:HB2	1.93	0.51
1:D:274:ASP:C	1:D:274:ASP:OD1	2.48	0.51
1:D:318:VAL:HG13	1:D:349:ALA:HB2	1.93	0.51
1:E:141:ILE:HG23	1:E:179:LEU:HD22	1.93	0.51
1:F:141:ILE:HG23	1:F:179:LEU:HD22	1.93	0.51
1:F:318:VAL:HG13	1:F:349:ALA:HB2	1.93	0.51
1:G:21:PHE:CD1	1:G:75:PHE:HE1	2.29	0.51
1:A:443:LEU:HA	1:A:460:ILE:HG12	1.93	0.51
1:B:165:LYS:NZ	3:B:602:ATP:O1G	2.40	0.51
1:D:156:PHE:HB2	1:D:287:PHE:CD1	2.46	0.51
1:D:399:MET:HE3	1:D:410:TRP:HA	1.92	0.51
1:E:205:THR:O	1:E:209:LEU:HG	2.11	0.51
1:H:49:THR:HG22	1:H:50:ARG:H	1.76	0.51
1:I:49:THR:HG22	1:I:50:ARG:H	1.76	0.51
1:I:77:TYR:CD1	1:I:77:TYR:O	2.64	0.51
1:A:74:PHE:CD2	1:A:77:TYR:HE2	2.29	0.51
1:A:192:ASP:HB3	1:A:251:ASP:O	2.11	0.51
1:A:207:ILE:O	1:A:208:LEU:C	2.49	0.51
1:E:438:SER:O	1:E:442:ALA:HA	2.11	0.51
1:F:269:LEU:HD22	1:F:270:VAL:H	1.75	0.51
1:F:274:ASP:C	1:F:274:ASP:OD1	2.48	0.51
1:F:310:PRO:HB3	1:F:316:GLU:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:529:PHE:N	1:F:530:PRO:CD	2.73	0.51
1:A:318:VAL:HG13	1:A:349:ALA:HB2	1.93	0.51
1:B:190:LEU:CD1	1:B:207:ILE:HG12	2.39	0.51
1:C:141:ILE:HG23	1:C:179:LEU:HD22	1.93	0.51
1:C:269:LEU:HD22	1:C:270:VAL:H	1.75	0.51
1:D:464:LEU:O	1:D:468:VAL:HG22	2.10	0.51
1:B:128:MET:HA	1:B:128:MET:CE	2.41	0.50
1:B:192:ASP:HB3	1:B:251:ASP:O	2.11	0.50
1:C:521:GLU:HG3	1:C:523:VAL:O	2.10	0.50
1:E:200:THR:HG21	1:E:256:GLU:HB3	1.93	0.50
1:G:23:PRO:HG2	1:G:53:ARG:HB3	1.93	0.50
1:A:156:PHE:HB2	1:A:287:PHE:CD1	2.46	0.50
1:B:24:ARG:NH2	1:B:53:ARG:HH11	2.09	0.50
1:C:233:ARG:NH1	1:C:237:ASN:HD21	2.09	0.50
1:C:485:LEU:HD12	1:C:486:GLU:N	2.25	0.50
1:D:438:SER:O	1:D:442:ALA:HA	2.11	0.50
1:H:77:TYR:CD1	1:H:77:TYR:O	2.64	0.50
1:A:211:LEU:HA	1:A:242:ARG:HH21	1.75	0.50
1:A:310:PRO:HA	1:A:345:PHE:HZ	1.76	0.50
1:C:192:ASP:HB3	1:C:251:ASP:O	2.11	0.50
1:D:141:ILE:HG23	1:D:179:LEU:HD22	1.93	0.50
1:D:250:ASP:HA	1:D:271:THR:OG1	2.11	0.50
1:E:157:LEU:HD11	1:E:168:ILE:HG22	1.92	0.50
1:E:269:LEU:HD22	1:E:270:VAL:H	1.75	0.50
1:E:459:ILE:HG13	1:E:460:ILE:H	1.77	0.50
1:E:318:VAL:CG1	1:E:349:ALA:HB2	2.42	0.50
1:B:184:TYR:HA	1:B:244:ASN:HB3	1.92	0.50
1:D:318:VAL:CG1	1:D:349:ALA:HB2	2.42	0.50
1:D:521:GLU:O	1:D:523:VAL:N	2.44	0.50
1:A:76:ASN:HA	1:A:81:SER:OG	2.12	0.50
1:A:318:VAL:CG1	1:A:349:ALA:HB2	2.42	0.50
1:B:156:PHE:HB2	1:B:287:PHE:CD1	2.46	0.50
1:D:327:SER:HB2	1:D:459:ILE:CD1	2.40	0.50
1:D:482:GLN:HB2	1:D:483:ARG:HD2	1.93	0.50
1:F:142:LYS:HE2	1:F:146:GLU:OE2	2.10	0.50
1:F:310:PRO:HD3	1:F:319:LEU:HD13	1.92	0.50
1:F:402:GLY:HA2	1:F:455:LYS:HD2	1.93	0.50
1:G:49:THR:HG22	1:G:50:ARG:H	1.76	0.50
1:B:262:GLN:HE22	1:B:282:SER:H	1.58	0.50
1:B:318:VAL:CG1	1:B:349:ALA:HB2	2.42	0.50
1:B:464:LEU:O	1:B:468:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HD11	1:C:87:LEU:CB	2.42	0.50
1:E:192:ASP:HB3	1:E:251:ASP:O	2.11	0.50
1:F:438:SER:O	1:F:442:ALA:HA	2.11	0.50
1:F:484:LEU:O	1:F:486:GLU:HG2	2.12	0.50
1:G:77:TYR:CD1	1:G:77:TYR:O	2.64	0.50
1:H:32:GLY:C	1:H:34:ASN:H	2.15	0.50
1:I:8:ARG:HH11	1:I:8:ARG:CG	2.14	0.50
1:A:250:ASP:HA	1:A:271:THR:OG1	2.11	0.50
1:B:187:ILE:HD13	1:B:246:LEU:HB3	1.92	0.50
1:B:250:ASP:HA	1:B:271:THR:OG1	2.12	0.50
1:C:283:GLN:HG3	1:E:126:LYS:NZ	2.26	0.50
1:F:192:ASP:HB3	1:F:251:ASP:O	2.11	0.50
1:F:250:ASP:HA	1:F:271:THR:OG1	2.11	0.50
1:B:397:VAL:HG21	1:B:468:VAL:HG11	1.93	0.50
1:C:310:PRO:HA	1:C:345:PHE:CZ	2.47	0.50
1:C:487:ILE:HB	1:C:531:LYS:HZ1	1.77	0.50
1:D:192:ASP:HB3	1:D:251:ASP:O	2.11	0.50
1:E:318:VAL:HG13	1:E:349:ALA:HB2	1.93	0.50
1:F:141:ILE:HG23	1:F:179:LEU:HD21	1.94	0.50
1:F:318:VAL:CG1	1:F:349:ALA:HB2	2.42	0.50
1:I:23:PRO:HG2	1:I:53:ARG:HB3	1.93	0.50
1:A:463:PHE:O	1:A:467:VAL:HB	2.12	0.49
1:B:443:LEU:HD22	1:B:460:ILE:HD11	1.94	0.49
1:C:29:TYR:O	1:C:33:LYS:HG3	2.12	0.49
1:C:58:LEU:O	1:C:62:ARG:HG3	2.12	0.49
1:D:155:LEU:HB3	1:D:269:LEU:HD23	1.94	0.49
1:B:318:VAL:HG13	1:B:349:ALA:HB2	1.93	0.49
1:B:445:SER:O	1:B:454:PHE:HA	2.12	0.49
1:C:37:THR:HG23	1:C:40:HIS:HD2	1.78	0.49
1:D:205:THR:O	1:D:209:LEU:HG	2.12	0.49
1:E:155:LEU:HB3	1:E:269:LEU:HD23	1.94	0.49
1:F:521:GLU:O	1:F:523:VAL:N	2.45	0.49
1:H:37:THR:H	1:H:40:HIS:HB2	1.78	0.49
1:I:35:ILE:CG2	1:I:35:ILE:O	2.60	0.49
1:A:438:SER:O	1:A:442:ALA:HA	2.11	0.49
1:A:483:ARG:HA	1:A:486:GLU:HG2	1.94	0.49
1:C:250:ASP:HA	1:C:271:THR:OG1	2.12	0.49
1:A:24:ARG:NH2	1:A:53:ARG:HH11	2.09	0.49
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.94	0.49
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.94	0.49
1:B:170:SER:O	1:B:174:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LEU:HB3	1:D:307:MET:HB3	1.95	0.49
1:F:162:GLY:O	1:F:330:PRO:HG2	2.11	0.49
1:F:399:MET:HE3	1:F:410:TRP:HA	1.94	0.49
1:F:456:ILE:HD13	1:F:461:HIS:HD2	1.77	0.49
1:F:484:LEU:HD13	1:F:533:MET:HG2	1.94	0.49
1:B:438:SER:O	1:B:442:ALA:HA	2.11	0.49
1:C:138:ASP:OD1	1:C:175:LYS:HE3	2.12	0.49
1:C:310:PRO:HG3	1:C:316:GLU:HA	1.93	0.49
1:C:405:ILE:HG12	1:C:410:TRP:CE3	2.48	0.49
1:E:206:ASP:O	1:E:210:MET:HG2	2.12	0.49
1:E:521:GLU:O	1:E:523:VAL:N	2.45	0.49
1:A:231:LEU:O	1:A:235:ILE:HG13	2.12	0.49
1:A:234:MET:CE	1:D:217:LEU:CD1	2.91	0.49
1:B:456:ILE:HD11	1:B:461:HIS:HA	1.95	0.49
1:B:484:LEU:HD22	1:B:533:MET:HG2	1.95	0.49
1:C:24:ARG:NH2	1:C:53:ARG:HH11	2.09	0.49
1:A:113:GLN:CD	1:A:113:GLN:H	2.16	0.49
1:A:262:GLN:NE2	1:A:283:GLN:HB2	2.28	0.49
1:A:327:SER:HB2	1:A:459:ILE:CD1	2.43	0.49
1:B:10:LEU:HD13	1:B:58:LEU:HD22	1.94	0.49
1:D:170:SER:O	1:D:174:SER:HB2	2.13	0.49
1:D:434:LEU:HB3	1:D:444:LEU:HD23	1.95	0.49
1:F:302:LEU:HB3	1:F:307:MET:HB3	1.95	0.49
1:A:521:GLU:O	1:A:523:VAL:N	2.45	0.49
1:B:1:MET:HE3	1:F:117:ARG:CZ	2.43	0.49
1:B:58:LEU:O	1:B:62:ARG:HG3	2.13	0.49
1:C:110:PHE:HB2	1:C:182:ILE:HD11	1.95	0.49
1:C:141:ILE:HG23	1:C:179:LEU:HD21	1.94	0.49
1:C:318:VAL:CG1	1:C:349:ALA:HB2	2.42	0.49
1:C:405:ILE:HB	1:C:525:ARG:HD2	1.95	0.49
1:E:128:MET:HA	1:E:128:MET:CE	2.43	0.49
1:E:250:ASP:HA	1:E:271:THR:OG1	2.11	0.49
1:E:302:LEU:HB3	1:E:307:MET:HB3	1.95	0.49
1:F:312:GLY:H	1:F:315:GLU:HB2	1.77	0.49
1:G:37:THR:H	1:G:40:HIS:HB2	1.77	0.49
1:A:106:ILE:HG22	1:A:182:ILE:HA	1.94	0.49
1:A:262:GLN:HE21	1:A:283:GLN:HB2	1.78	0.49
1:D:378:LEU:O	1:D:379:GLN:C	2.52	0.49
1:E:262:GLN:HE21	1:E:283:GLN:HB2	1.76	0.49
3:A:602:ATP:H2'	3:A:602:ATP:N3	2.28	0.49
1:C:259:ARG:O	1:C:263:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LEU:HD12	1:E:207:ILE:HG12	1.94	0.48
1:E:484:LEU:CD1	1:E:533:MET:HG2	2.41	0.48
1:A:141:ILE:HD12	1:A:175:LYS:HZ2	1.78	0.48
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.94	0.48
1:A:170:SER:O	1:A:174:SER:HB2	2.13	0.48
1:B:236:CYS:SG	1:F:121:LEU:HD23	2.53	0.48
1:B:524:ILE:HA	1:B:525:ARG:HH21	1.78	0.48
1:C:479:ILE:HG23	1:C:483:ARG:NH2	2.28	0.48
1:D:405:ILE:HG12	1:D:410:TRP:CE3	2.48	0.48
1:E:141:ILE:HG23	1:E:179:LEU:HD21	1.94	0.48
1:E:452:LEU:H	1:E:452:LEU:CD2	2.23	0.48
1:F:239:LEU:O	1:F:239:LEU:HD13	2.13	0.48
1:F:255:GLU:HB3	1:F:277:ILE:HG22	1.94	0.48
1:H:24:ARG:NH2	1:H:53:ARG:HH11	2.11	0.48
1:H:37:THR:O	1:H:40:HIS:HB2	2.13	0.48
1:A:58:LEU:O	1:A:62:ARG:HG3	2.13	0.48
1:D:347:LYS:NZ	1:D:351:LEU:HD21	2.28	0.48
3:E:602:ATP:N3	3:E:602:ATP:H2'	2.28	0.48
1:F:131:TYR:CD1	1:F:131:TYR:C	2.87	0.48
1:F:155:LEU:HB3	1:F:269:LEU:HD23	1.94	0.48
1:F:460:ILE:O	1:F:464:LEU:HG	2.13	0.48
1:H:35:ILE:O	1:H:35:ILE:CG2	2.60	0.48
1:I:37:THR:H	1:I:40:HIS:HB2	1.77	0.48
1:A:29:TYR:CZ	1:A:33:LYS:HD2	2.48	0.48
1:A:302:LEU:HB3	1:A:307:MET:HB3	1.95	0.48
1:A:405:ILE:HG12	1:A:410:TRP:CE3	2.48	0.48
1:B:347:LYS:NZ	1:B:351:LEU:HD21	2.28	0.48
1:C:155:LEU:HB3	1:C:269:LEU:HD23	1.94	0.48
1:C:165:LYS:NZ	3:C:602:ATP:O1G	2.40	0.48
1:C:391:SER:O	1:C:392:ALA:C	2.50	0.48
1:C:399:MET:HE3	1:C:409:LEU:O	2.14	0.48
3:C:602:ATP:H2'	3:C:602:ATP:N3	2.28	0.48
1:F:208:LEU:CB	1:F:235:ILE:HG12	2.34	0.48
1:I:37:THR:O	1:I:40:HIS:HB2	2.13	0.48
1:A:49:THR:HG22	1:A:50:ARG:N	2.29	0.48
1:A:252:VAL:HG11	1:A:258:ILE:CD1	2.44	0.48
1:B:302:LEU:HB3	1:B:307:MET:HB3	1.95	0.48
1:B:452:LEU:H	1:B:452:LEU:CD2	2.23	0.48
1:C:302:LEU:HB3	1:C:307:MET:HB3	1.95	0.48
1:D:127:GLN:OE1	1:D:171:GLN:HA	2.13	0.48
1:E:340:CYS:HA	1:E:347:LYS:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:ILE:HG12	1:E:410:TRP:CE3	2.48	0.48
1:F:347:LYS:NZ	1:F:351:LEU:HD21	2.28	0.48
1:G:32:GLY:C	1:G:34:ASN:H	2.15	0.48
1:I:24:ARG:NH2	1:I:53:ARG:HH11	2.11	0.48
1:I:32:GLY:C	1:I:34:ASN:H	2.15	0.48
1:A:347:LYS:NZ	1:A:351:LEU:HD21	2.28	0.48
1:B:334:MET:HA	1:B:337:PHE:CD2	2.49	0.48
1:C:204:PHE:O	1:C:235:ILE:HD11	2.14	0.48
1:C:302:LEU:HD23	1:C:337:PHE:HE1	1.77	0.48
1:C:378:LEU:O	1:C:379:GLN:C	2.52	0.48
1:D:253:VAL:HG11	1:D:380:ARG:CZ	2.44	0.48
1:E:262:GLN:NE2	1:E:283:GLN:HB2	2.28	0.48
1:F:378:LEU:O	1:F:379:GLN:C	2.52	0.48
1:F:399:MET:HG3	1:F:410:TRP:NE1	2.28	0.48
1:F:405:ILE:HG12	1:F:410:TRP:CE3	2.48	0.48
1:G:37:THR:O	1:G:40:HIS:HB2	2.13	0.48
1:A:283:GLN:HG2	1:A:284:THR:N	2.26	0.48
1:B:49:THR:HG22	1:B:50:ARG:N	2.29	0.48
1:C:347:LYS:NZ	1:C:351:LEU:HD21	2.28	0.48
1:G:35:ILE:CG2	1:G:35:ILE:O	2.60	0.48
1:G:58:LEU:O	1:G:62:ARG:HG3	2.14	0.48
1:H:58:LEU:O	1:H:62:ARG:HG3	2.14	0.48
1:A:393:LEU:CD2	1:A:464:LEU:HD11	2.44	0.48
1:B:141:ILE:HG23	1:B:179:LEU:HD21	1.94	0.48
1:B:207:ILE:O	1:B:211:LEU:HG	2.14	0.48
1:B:478:SER:O	1:B:482:GLN:HG2	2.13	0.48
1:B:485:LEU:HD12	1:B:486:GLU:N	2.28	0.48
1:C:21:PHE:CD1	1:C:75:PHE:CE1	3.02	0.48
1:C:131:TYR:CD1	1:C:131:TYR:C	2.87	0.48
1:C:178:GLN:HA	1:C:182:ILE:HB	1.95	0.48
1:D:141:ILE:HG23	1:D:179:LEU:HD21	1.94	0.48
1:F:259:ARG:O	1:F:263:GLU:HG3	2.13	0.48
1:A:141:ILE:HG23	1:A:179:LEU:HD21	1.94	0.48
1:B:306:GLY:O	1:B:343:LYS:HD3	2.14	0.48
1:C:10:LEU:HD13	1:C:58:LEU:HD22	1.94	0.48
1:C:347:LYS:O	1:C:351:LEU:HG	2.14	0.48
1:D:208:LEU:O	1:D:212:LYS:HG2	2.13	0.48
1:E:131:TYR:CD1	1:E:131:TYR:C	2.87	0.48
1:E:463:PHE:HD2	1:E:464:LEU:HD23	1.78	0.48
1:F:115:LEU:HD23	1:F:115:LEU:HA	1.53	0.48
1:F:311:VAL:HB	1:F:315:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:VAL:HG21	1:F:468:VAL:HG21	1.96	0.48
1:A:10:LEU:HD13	1:A:58:LEU:HD22	1.94	0.48
1:B:160:ARG:HG2	1:B:161:ALA:H	1.78	0.48
1:E:378:LEU:O	1:E:379:GLN:C	2.52	0.48
1:F:452:LEU:H	1:F:452:LEU:CD2	2.23	0.48
1:A:158:HIS:ND1	1:A:158:HIS:O	2.47	0.47
1:B:141:ILE:HG23	1:B:179:LEU:HD22	1.93	0.47
1:B:487:ILE:HB	1:B:531:LYS:NZ	2.28	0.47
1:C:49:THR:HG22	1:C:50:ARG:N	2.29	0.47
1:C:329:ASN:HD22	1:C:330:PRO:HD2	1.78	0.47
1:D:158:HIS:NE2	1:D:287:PHE:HB3	2.29	0.47
1:D:212:LYS:NZ	1:D:238:ALA:HB2	2.28	0.47
1:E:347:LYS:O	1:E:350:GLN:HB2	2.14	0.47
1:F:325:LEU:O	1:F:459:ILE:HG23	2.13	0.47
1:G:88:GLU:O	1:G:91:ILE:HG22	2.14	0.47
1:A:32:GLY:C	1:A:34:ASN:H	2.17	0.47
1:A:444:LEU:HD12	1:A:454:PHE:HB3	1.96	0.47
3:D:602:ATP:H2'	3:D:602:ATP:N3	2.28	0.47
1:H:88:GLU:O	1:H:91:ILE:HG22	2.14	0.47
1:A:37:THR:HG23	1:A:40:HIS:HD2	1.79	0.47
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.14	0.47
1:B:77:TYR:CD1	1:B:77:TYR:O	2.67	0.47
1:B:112:ARG:CZ	1:B:115:LEU:HD12	2.44	0.47
1:B:212:LYS:HA	1:B:212:LYS:CE	2.30	0.47
1:B:405:ILE:HG12	1:B:410:TRP:CE3	2.48	0.47
1:C:76:ASN:HA	1:C:81:SER:OG	2.14	0.47
1:C:77:TYR:CD1	1:C:77:TYR:O	2.67	0.47
1:C:177:ASP:O	1:C:178:GLN:C	2.50	0.47
1:C:526:PRO:HB3	1:C:529:PHE:HD2	1.79	0.47
1:E:344:THR:HG22	1:E:346:GLU:H	1.78	0.47
1:F:203:LEU:O	1:F:207:ILE:HG13	2.14	0.47
1:F:363:VAL:O	1:F:363:VAL:HG13	2.14	0.47
1:A:327:SER:HB2	1:A:459:ILE:CG1	2.44	0.47
1:A:466:HIS:N	1:A:466:HIS:ND1	2.62	0.47
1:B:102:ARG:HA	1:B:106:ILE:HB	1.96	0.47
1:D:363:VAL:O	1:D:363:VAL:HG13	2.14	0.47
1:D:452:LEU:H	1:D:452:LEU:CD2	2.23	0.47
1:E:330:PRO:HB3	3:E:602:ATP:C8	2.50	0.47
1:E:363:VAL:O	1:E:363:VAL:HG13	2.14	0.47
1:A:190:LEU:HD12	1:A:207:ILE:CG1	2.43	0.47
1:A:347:LYS:O	1:A:351:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PHE:HA	1:B:207:ILE:HG13	1.95	0.47
3:B:602:ATP:N3	3:B:602:ATP:H2'	2.28	0.47
1:D:161:ALA:HA	1:D:273:ARG:HD3	1.96	0.47
1:H:22:GLU:OE2	1:H:24:ARG:HG3	2.15	0.47
1:A:88:GLU:O	1:A:91:ILE:HG22	2.15	0.47
1:B:131:TYR:CD1	1:B:131:TYR:C	2.87	0.47
1:B:378:LEU:O	1:B:379:GLN:C	2.52	0.47
1:C:72:ILE:HG21	1:C:88:GLU:HG3	1.97	0.47
1:D:310:PRO:HA	1:D:345:PHE:CZ	2.50	0.47
1:F:255:GLU:CB	1:F:277:ILE:HG22	2.45	0.47
1:G:22:GLU:OE2	1:G:24:ARG:HG3	2.15	0.47
1:I:88:GLU:O	1:I:91:ILE:HG22	2.14	0.47
1:A:4:GLU:HG3	1:A:5:ILE:N	2.29	0.47
1:A:131:TYR:C	1:A:131:TYR:CD1	2.87	0.47
1:B:21:PHE:CD1	1:B:75:PHE:CE1	3.02	0.47
1:B:88:GLU:O	1:B:91:ILE:HG22	2.15	0.47
1:B:307:MET:SD	1:B:343:LYS:HG3	2.55	0.47
1:B:406:PRO:HD3	1:B:524:ILE:HD11	1.96	0.47
1:C:88:GLU:O	1:C:91:ILE:HG22	2.15	0.47
1:C:158:HIS:ND1	1:C:158:HIS:O	2.47	0.47
1:C:343:LYS:HE3	1:C:343:LYS:HB3	1.75	0.47
1:D:239:LEU:O	1:D:239:LEU:HD13	2.15	0.47
1:D:399:MET:HG3	1:D:410:TRP:NE1	2.30	0.47
1:E:321:LYS:O	1:E:325:LEU:HG	2.15	0.47
1:F:398:VAL:CG2	1:F:413:VAL:HG11	2.36	0.47
1:G:8:ARG:HH11	1:G:8:ARG:CG	2.14	0.47
1:G:24:ARG:NH2	1:G:53:ARG:HH11	2.11	0.47
1:G:35:ILE:HG22	1:G:36:PHE:HD1	1.80	0.47
1:A:205:THR:HA	1:A:231:LEU:HD11	1.96	0.47
1:B:67:GLU:HG2	1:B:69:GLY:H	1.79	0.47
1:B:76:ASN:HA	1:B:81:SER:OG	2.14	0.47
1:B:327:SER:HB2	1:B:459:ILE:CG1	2.44	0.47
1:B:436:ARG:O	1:B:440:ARG:HG3	2.15	0.47
1:C:165:LYS:HG2	1:C:290:VAL:HG21	1.97	0.47
1:E:343:LYS:HG2	1:E:343:LYS:O	2.14	0.47
1:F:347:LYS:O	1:F:351:LEU:HG	2.14	0.47
1:G:21:PHE:CD1	1:G:75:PHE:CE1	3.03	0.47
1:I:72:ILE:C	1:I:74:PHE:H	2.18	0.47
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.45	0.47
1:A:330:PRO:HB3	3:A:602:ATP:C8	2.50	0.47
1:B:165:LYS:HG3	3:B:602:ATP:O2B	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLU:HG3	1:C:5:ILE:N	2.30	0.47
1:C:159:GLY:H	1:C:165:LYS:HD3	1.77	0.47
1:G:4:GLU:HG3	1:G:5:ILE:N	2.30	0.47
1:A:204:PHE:HA	1:A:207:ILE:HD12	1.96	0.47
1:B:22:GLU:HG3	1:B:24:ARG:H	1.80	0.47
1:C:398:VAL:HG12	1:C:540:TYR:OH	2.15	0.47
1:D:165:LYS:HG3	3:D:602:ATP:O2B	2.15	0.47
1:H:35:ILE:HG22	1:H:36:PHE:HD1	1.80	0.47
1:A:115:LEU:CD1	1:A:177:ASP:HA	2.45	0.46
1:A:378:LEU:O	1:A:379:GLN:C	2.52	0.46
1:B:160:ARG:HG2	1:B:161:ALA:N	2.30	0.46
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.97	0.46
1:B:481:GLU:HA	1:B:484:LEU:HB3	1.95	0.46
1:C:482:GLN:HB2	1:C:483:ARG:HH21	1.80	0.46
1:D:436:ARG:O	1:D:440:ARG:HG3	2.15	0.46
3:F:602:ATP:H2'	3:F:602:ATP:N3	2.28	0.46
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.97	0.46
1:B:307:MET:HA	1:B:308:PRO:HD3	1.82	0.46
1:B:347:LYS:O	1:B:351:LEU:HG	2.14	0.46
1:C:255:GLU:HB3	1:C:277:ILE:HG22	1.96	0.46
1:D:127:GLN:HE22	1:D:171:GLN:HG2	1.80	0.46
1:D:347:LYS:O	1:D:351:LEU:HG	2.14	0.46
1:E:160:ARG:HG2	1:E:161:ALA:H	1.79	0.46
1:E:165:LYS:HG2	1:E:290:VAL:HG21	1.97	0.46
1:E:253:VAL:HG11	1:E:380:ARG:CZ	2.46	0.46
1:F:436:ARG:O	1:F:440:ARG:HG3	2.15	0.46
1:I:58:LEU:O	1:I:62:ARG:HG3	2.14	0.46
1:A:208:LEU:HD23	1:A:235:ILE:HA	1.96	0.46
1:C:160:ARG:HG2	1:C:161:ALA:N	2.31	0.46
1:C:298:CYS:O	1:C:302:LEU:HD12	2.16	0.46
1:D:460:ILE:HD12	1:D:460:ILE:HA	1.80	0.46
1:E:340:CYS:HA	1:E:347:LYS:HE3	1.96	0.46
1:E:436:ARG:O	1:E:440:ARG:HG3	2.15	0.46
1:F:161:ALA:C	1:F:163:SER:H	2.19	0.46
1:H:72:ILE:HG21	1:H:88:GLU:CG	2.46	0.46
1:I:35:ILE:HG22	1:I:36:PHE:HD1	1.80	0.46
1:A:22:GLU:HG3	1:A:24:ARG:H	1.80	0.46
1:A:363:VAL:O	1:A:363:VAL:HG13	2.15	0.46
1:A:452:LEU:H	1:A:452:LEU:CD2	2.23	0.46
1:A:462:MET:HB2	1:A:462:MET:HE3	1.52	0.46
1:B:107:ALA:O	1:B:110:PHE:HD1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASN:ND2	1:F:214:GLU:HG3	2.31	0.46
1:D:321:LYS:O	1:D:325:LEU:HG	2.15	0.46
1:E:143:LYS:O	1:E:147:MET:HE3	2.15	0.46
1:E:165:LYS:HG3	3:E:602:ATP:O2B	2.15	0.46
1:E:366:ILE:H	1:E:366:ILE:CD1	2.20	0.46
1:F:143:LYS:O	1:F:147:MET:HE3	2.16	0.46
1:F:160:ARG:HG2	1:F:161:ALA:H	1.79	0.46
1:H:21:PHE:CD1	1:H:75:PHE:CE1	3.03	0.46
1:A:298:CYS:O	1:A:302:LEU:HD12	2.16	0.46
1:A:399:MET:HG3	1:A:410:TRP:NE1	2.30	0.46
1:B:298:CYS:O	1:B:302:LEU:HD12	2.16	0.46
1:C:22:GLU:HG3	1:C:24:ARG:H	1.80	0.46
1:C:465:LYS:C	1:C:467:VAL:H	2.19	0.46
1:C:483:ARG:HD2	1:C:483:ARG:N	2.30	0.46
1:D:160:ARG:HG2	1:D:161:ALA:H	1.81	0.46
1:F:302:LEU:HD23	1:F:337:PHE:HE1	1.77	0.46
1:I:22:GLU:OE2	1:I:24:ARG:HG3	2.15	0.46
1:A:201:PHE:CD1	1:A:201:PHE:C	2.89	0.46
1:A:436:ARG:O	1:A:440:ARG:HG3	2.15	0.46
1:B:124:VAL:HA	1:B:125:PRO:HD3	1.68	0.46
1:B:483:ARG:N	1:B:483:ARG:HD2	2.30	0.46
1:B:526:PRO:HB2	1:B:529:PHE:CD2	2.50	0.46
1:C:165:LYS:HG3	3:C:602:ATP:O2B	2.15	0.46
1:E:204:PHE:CZ	1:E:260:TRP:HB3	2.51	0.46
1:H:72:ILE:C	1:H:74:PHE:H	2.18	0.46
1:A:252:VAL:HG12	1:A:277:ILE:HD13	1.98	0.46
1:A:283:GLN:HG3	1:D:126:LYS:NZ	2.30	0.46
1:C:207:ILE:O	1:C:211:LEU:HG	2.15	0.46
1:C:275:VAL:O	1:C:275:VAL:HG12	2.16	0.46
1:A:341:GLU:OE2	1:A:342:PRO:HD3	2.16	0.46
1:A:456:ILE:CG1	1:A:460:ILE:CG2	2.92	0.46
1:B:201:PHE:CD1	1:B:201:PHE:C	2.89	0.46
1:B:321:LYS:O	1:B:325:LEU:HG	2.15	0.46
1:C:205:THR:HA	1:C:231:LEU:HD11	1.96	0.46
1:C:240:ILE:C	1:C:242:ARG:H	2.19	0.46
1:C:406:PRO:HD3	1:C:525:ARG:HB2	1.97	0.46
1:D:252:VAL:HG12	1:D:277:ILE:HD13	1.98	0.46
1:D:478:SER:O	1:D:482:GLN:HG2	2.15	0.46
1:F:165:LYS:HG2	1:F:290:VAL:HG21	1.97	0.46
1:I:4:GLU:HG3	1:I:5:ILE:N	2.30	0.46
1:I:21:PHE:CD1	1:I:75:PHE:CE1	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ALA:HB2	1:B:90:TYR:CD1	2.51	0.46
1:E:201:PHE:CD1	1:E:201:PHE:C	2.89	0.46
1:F:298:CYS:O	1:F:302:LEU:HD12	2.16	0.46
1:G:92:ASP:C	1:G:94:ALA:H	2.19	0.46
1:A:30:LEU:CD2	1:A:35:ILE:HG13	2.40	0.46
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.35	0.46
1:B:23:PRO:HG2	1:B:53:ARG:CB	2.46	0.46
1:B:336:PHE:HE2	1:B:351:LEU:HB2	1.81	0.46
1:C:22:GLU:OE2	1:C:24:ARG:HG3	2.16	0.46
1:C:23:PRO:HG2	1:C:53:ARG:CB	2.46	0.46
1:F:252:VAL:HG12	1:F:277:ILE:HD13	1.98	0.46
1:A:23:PRO:HG2	1:A:53:ARG:CB	2.46	0.45
1:A:399:MET:HE3	1:A:410:TRP:HA	1.98	0.45
1:B:412:CYS:HB3	1:B:483:ARG:HB2	1.98	0.45
1:B:532:PHE:C	1:B:534:GLN:N	2.70	0.45
1:C:116:ASP:N	1:C:116:ASP:OD1	2.49	0.45
1:C:262:GLN:OE1	1:C:281:ALA:HA	2.15	0.45
1:D:275:VAL:O	1:D:275:VAL:HG12	2.16	0.45
1:D:342:PRO:C	1:D:344:THR:H	2.20	0.45
1:E:252:VAL:HG12	1:E:277:ILE:HD13	1.98	0.45
1:F:165:LYS:HG3	3:F:602:ATP:O2B	2.15	0.45
1:H:4:GLU:HG3	1:H:5:ILE:N	2.30	0.45
1:A:62:ARG:HD2	1:A:241:ASP:OD1	2.16	0.45
1:A:165:LYS:HG3	3:A:602:ATP:O2B	2.15	0.45
1:B:121:LEU:CD2	1:D:233:ARG:CD	2.94	0.45
1:B:310:PRO:HA	1:B:345:PHE:CZ	2.51	0.45
1:C:283:GLN:HG2	1:C:284:THR:N	2.31	0.45
1:D:143:LYS:O	1:D:147:MET:HE3	2.15	0.45
1:D:165:LYS:HG2	1:D:290:VAL:HG21	1.97	0.45
1:D:484:LEU:HD11	1:D:533:MET:H	1.82	0.45
1:B:363:VAL:HG13	1:B:363:VAL:O	2.14	0.45
1:C:8:ARG:HA	1:C:243:PRO:HG3	1.97	0.45
1:C:452:LEU:H	1:C:452:LEU:CD2	2.23	0.45
1:D:160:ARG:HG2	1:D:161:ALA:N	2.30	0.45
1:E:298:CYS:O	1:E:302:LEU:HD12	2.16	0.45
1:F:247:PHE:CE2	1:F:266:LEU:HD22	2.51	0.45
1:H:92:ASP:C	1:H:94:ALA:H	2.20	0.45
1:A:9:ALA:HB2	1:A:90:TYR:CD1	2.51	0.45
1:A:302:LEU:HD23	1:A:337:PHE:HE1	1.77	0.45
1:A:459:ILE:H	1:A:459:ILE:HG13	1.41	0.45
1:B:22:GLU:OE2	1:B:24:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HG21	1:C:182:ILE:HA	1.98	0.45
1:C:201:PHE:CD1	1:C:201:PHE:C	2.89	0.45
1:C:252:VAL:HG12	1:C:277:ILE:HD13	1.98	0.45
1:D:116:ASP:OD1	1:D:116:ASP:N	2.49	0.45
1:E:275:VAL:O	1:E:275:VAL:HG12	2.16	0.45
1:E:463:PHE:CD2	1:E:464:LEU:HD23	2.51	0.45
1:F:177:ASP:O	1:F:182:ILE:HD13	2.16	0.45
1:C:9:ALA:HB2	1:C:90:TYR:CD1	2.51	0.45
1:C:252:VAL:HG11	1:C:258:ILE:CD1	2.43	0.45
1:C:363:VAL:O	1:C:363:VAL:HG13	2.14	0.45
1:C:401:PRO:HA	1:C:456:ILE:O	2.17	0.45
1:I:92:ASP:C	1:I:94:ALA:H	2.20	0.45
1:B:252:VAL:HG12	1:B:277:ILE:HD13	1.98	0.45
1:C:265:ARG:HH21	1:E:126:LYS:N	2.14	0.45
1:C:532:PHE:C	1:C:534:GLN:N	2.70	0.45
1:E:525:ARG:HA	1:E:526:PRO:HD3	1.71	0.45
1:A:61:TYR:CE1	1:A:71:LEU:HD23	2.51	0.45
1:A:275:VAL:O	1:A:275:VAL:HG12	2.16	0.45
1:E:155:LEU:HD23	1:E:155:LEU:HA	1.77	0.45
1:E:329:ASN:HB3	1:E:332:THR:OG1	2.16	0.45
1:F:162:GLY:C	1:F:164:GLY:N	2.70	0.45
1:F:184:TYR:HB3	1:F:244:ASN:O	2.15	0.45
1:F:201:PHE:CD1	1:F:201:PHE:C	2.89	0.45
1:H:9:ALA:HB2	1:H:90:TYR:CD1	2.52	0.45
1:H:97:GLU:HA	1:H:98:PRO:HD3	1.73	0.45
1:A:22:GLU:OE2	1:A:24:ARG:HG3	2.16	0.45
1:A:109:GLN:OE1	1:A:109:GLN:N	2.50	0.45
1:A:237:ASN:C	1:A:239:LEU:H	2.19	0.45
1:A:343:LYS:HB3	1:A:343:LYS:HE2	1.52	0.45
1:A:371:TYR:CD2	1:A:377:ALA:HB2	2.52	0.45
1:B:116:ASP:OD1	1:B:116:ASP:N	2.49	0.45
1:D:206:ASP:O	1:D:210:MET:HG2	2.17	0.45
1:D:298:CYS:O	1:D:302:LEU:HD12	2.16	0.45
1:E:371:TYR:CD2	1:E:377:ALA:HB2	2.52	0.45
1:F:371:TYR:CD2	1:F:377:ALA:HB2	2.52	0.45
1:I:2:LEU:O	1:I:3:CYS:HB3	2.17	0.45
1:I:97:GLU:HA	1:I:98:PRO:HD3	1.73	0.45
1:A:163:SER:C	1:A:330:PRO:HG2	2.37	0.45
1:C:2:LEU:HB3	1:C:6:GLU:HB2	1.98	0.45
1:C:478:SER:HA	1:C:481:GLU:CD	2.37	0.45
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:HG22	1:D:269:LEU:HD12	1.99	0.45
1:E:341:GLU:N	1:E:342:PRO:HD2	2.32	0.45
1:E:535:LEU:O	1:E:535:LEU:HD23	2.17	0.45
1:F:534:GLN:HE21	1:F:534:GLN:CA	2.19	0.45
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.52	0.45
1:B:121:LEU:HD22	1:D:233:ARG:CD	2.46	0.45
1:B:121:LEU:HD23	1:D:233:ARG:HD2	1.99	0.45
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.80	0.45
1:C:162:GLY:O	1:C:330:PRO:HG2	2.16	0.45
1:C:259:ARG:HG2	1:C:280:ALA:HB1	2.00	0.45
1:F:405:ILE:HA	1:F:406:PRO:HD3	1.82	0.45
1:G:97:GLU:HA	1:G:98:PRO:HD3	1.73	0.45
1:A:234:MET:HE2	1:D:217:LEU:CD1	2.42	0.44
1:B:535:LEU:O	1:B:535:LEU:HD23	2.17	0.44
1:C:321:LYS:O	1:C:325:LEU:HG	2.17	0.44
1:D:115:LEU:HD11	1:D:177:ASP:HA	1.98	0.44
1:D:204:PHE:CG	1:D:207:ILE:HD12	2.53	0.44
1:D:371:TYR:CD2	1:D:377:ALA:HB2	2.52	0.44
1:D:532:PHE:C	1:D:534:GLN:N	2.70	0.44
1:E:135:TYR:CZ	1:E:139:ARG:HD2	2.52	0.44
1:E:161:ALA:C	1:E:163:SER:H	2.21	0.44
1:F:275:VAL:O	1:F:275:VAL:HG12	2.16	0.44
1:F:540:TYR:O	1:F:543:LEU:HD23	2.17	0.44
1:G:9:ALA:HB2	1:G:90:TYR:CD1	2.52	0.44
1:A:183:ASN:O	1:A:244:ASN:ND2	2.50	0.44
1:B:248:VAL:HG22	1:B:269:LEU:HD12	1.99	0.44
1:D:315:GLU:HB3	1:D:345:PHE:CE2	2.52	0.44
1:B:540:TYR:O	1:B:543:LEU:HD23	2.17	0.44
1:C:141:ILE:HD11	1:C:175:LYS:HB3	2.00	0.44
1:C:374:LEU:HD13	1:C:378:LEU:HG	1.99	0.44
1:D:162:GLY:O	1:D:330:PRO:HG2	2.18	0.44
1:D:274:ASP:O	1:D:277:ILE:HG12	2.18	0.44
1:D:329:ASN:HD22	1:D:330:PRO:HD2	1.82	0.44
1:D:535:LEU:HD23	1:D:535:LEU:O	2.17	0.44
1:E:204:PHE:CD2	1:E:207:ILE:HD12	2.52	0.44
1:E:284:THR:HG22	1:E:286:GLU:OE1	2.17	0.44
1:E:390:ARG:HE	1:E:390:ARG:HB2	1.61	0.44
1:F:128:MET:HA	1:F:128:MET:CE	2.47	0.44
1:F:188:VAL:HB	1:F:247:PHE:HD1	1.82	0.44
1:H:2:LEU:O	1:H:3:CYS:HB3	2.17	0.44
1:B:67:GLU:HG2	1:B:68:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:MET:HA	1:B:128:MET:HE2	1.98	0.44
1:B:459:ILE:H	1:B:459:ILE:HG13	1.41	0.44
1:C:535:LEU:O	1:C:535:LEU:HD23	2.17	0.44
1:D:201:PHE:C	1:D:201:PHE:CD1	2.89	0.44
1:D:527:GLU:N	1:D:527:GLU:OE1	2.51	0.44
1:E:248:VAL:HG22	1:E:269:LEU:HD12	1.99	0.44
1:F:262:GLN:HE22	1:F:282:SER:H	1.65	0.44
1:F:478:SER:HA	1:F:481:GLU:CD	2.38	0.44
1:A:67:GLU:HG2	1:A:68:LEU:N	2.33	0.44
1:A:401:PRO:HA	1:A:456:ILE:O	2.18	0.44
1:B:121:LEU:CD2	1:D:233:ARG:HD2	2.47	0.44
1:C:171:GLN:O	1:C:175:LYS:N	2.47	0.44
1:C:274:ASP:O	1:C:277:ILE:HG12	2.18	0.44
1:E:237:ASN:O	1:E:240:ILE:HG12	2.17	0.44
1:E:393:LEU:HB2	1:E:437:LEU:HD11	2.00	0.44
1:F:116:ASP:N	1:F:116:ASP:OD1	2.49	0.44
1:F:240:ILE:C	1:F:242:ARG:H	2.21	0.44
1:F:532:PHE:C	1:F:534:GLN:N	2.70	0.44
1:A:274:ASP:O	1:A:277:ILE:HG12	2.18	0.44
1:D:478:SER:HA	1:D:481:GLU:CD	2.37	0.44
1:D:540:TYR:O	1:D:543:LEU:HD23	2.18	0.44
1:E:185:ASP:H	1:E:244:ASN:CB	2.31	0.44
1:E:540:TYR:O	1:E:543:LEU:HD23	2.18	0.44
1:F:481:GLU:O	1:F:484:LEU:HB3	2.17	0.44
1:G:72:ILE:CD1	1:G:87:LEU:HB2	2.48	0.44
1:B:237:ASN:O	1:B:240:ILE:HG12	2.18	0.44
1:B:521:GLU:HG3	1:B:523:VAL:O	2.17	0.44
1:C:273:ARG:NH2	1:C:380:ARG:HH21	2.16	0.44
1:D:135:TYR:CZ	1:D:139:ARG:HD2	2.52	0.44
1:D:302:LEU:CD2	1:D:337:PHE:HE1	2.31	0.44
1:D:525:ARG:HH11	1:D:535:LEU:HD13	1.83	0.44
1:F:374:LEU:HD13	1:F:378:LEU:HG	1.99	0.44
1:I:9:ALA:HB2	1:I:90:TYR:CD1	2.52	0.44
1:I:29:TYR:OH	1:I:33:LYS:HD2	2.18	0.44
1:I:35:ILE:O	1:I:36:PHE:HD1	2.01	0.44
1:A:211:LEU:CD1	1:A:239:LEU:HD23	2.45	0.44
1:A:248:VAL:HG22	1:A:269:LEU:HD12	1.99	0.44
1:A:525:ARG:HH11	1:A:535:LEU:HD13	1.83	0.44
1:A:535:LEU:HD23	1:A:535:LEU:O	2.17	0.44
1:B:143:LYS:O	1:B:147:MET:HE3	2.18	0.44
1:B:275:VAL:O	1:B:275:VAL:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:O	1:C:115:LEU:HB2	2.17	0.44
1:C:248:VAL:HG22	1:C:269:LEU:HD12	1.99	0.44
1:C:426:LEU:HD23	1:C:426:LEU:HA	1.75	0.44
1:D:154:PHE:HE2	1:D:262:GLN:HG3	1.83	0.44
1:D:247:PHE:CE2	1:D:266:LEU:HD22	2.53	0.44
1:E:310:PRO:CB	1:E:316:GLU:HB3	2.47	0.44
1:E:525:ARG:HH11	1:E:535:LEU:HD13	1.83	0.44
1:F:135:TYR:CZ	1:F:139:ARG:HD2	2.52	0.44
1:F:535:LEU:O	1:F:535:LEU:HD23	2.17	0.44
1:A:400:PRO:HD3	1:A:540:TYR:HE1	1.83	0.44
1:A:540:TYR:O	1:A:543:LEU:HD23	2.18	0.44
1:B:208:LEU:HD21	1:B:234:MET:HG2	2.00	0.44
1:B:374:LEU:HD13	1:B:378:LEU:HG	1.99	0.44
1:C:371:TYR:CD2	1:C:377:ALA:HB2	2.52	0.44
1:F:302:LEU:CD2	1:F:337:PHE:HE1	2.31	0.44
1:F:527:GLU:N	1:F:527:GLU:OE1	2.51	0.44
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.79	0.43
1:B:72:ILE:HG21	1:B:88:GLU:HG3	1.99	0.43
1:C:302:LEU:CD2	1:C:337:PHE:HE1	2.31	0.43
1:E:163:SER:O	1:E:330:PRO:HG2	2.18	0.43
1:E:302:LEU:CD2	1:E:337:PHE:HE1	2.31	0.43
1:F:274:ASP:O	1:F:277:ILE:HG12	2.18	0.43
1:A:8:ARG:CG	1:A:8:ARG:NH1	2.74	0.43
1:B:274:ASP:O	1:B:277:ILE:HG12	2.18	0.43
1:C:158:HIS:CD2	1:C:287:PHE:HB3	2.54	0.43
1:D:456:ILE:HD13	1:D:461:HIS:HD2	1.82	0.43
1:E:273:ARG:NH2	1:E:380:ARG:HH21	2.16	0.43
1:E:374:LEU:HD13	1:E:378:LEU:HG	1.99	0.43
1:E:527:GLU:OE1	1:E:527:GLU:N	2.51	0.43
1:F:525:ARG:HH11	1:F:535:LEU:HD13	1.83	0.43
1:H:29:TYR:OH	1:H:33:LYS:HD2	2.18	0.43
1:B:128:MET:HB2	1:B:171:GLN:NE2	2.34	0.43
1:B:371:TYR:CD2	1:B:377:ALA:HB2	2.52	0.43
1:B:487:ILE:HB	1:B:531:LYS:HZ1	1.82	0.43
1:C:445:SER:O	1:C:454:PHE:HA	2.18	0.43
1:D:469:ASP:OD2	1:D:471:GLN:HB3	2.18	0.43
1:E:163:SER:C	1:E:330:PRO:HG2	2.37	0.43
1:E:302:LEU:HD23	1:E:337:PHE:HE1	1.77	0.43
1:F:160:ARG:HG2	1:F:161:ALA:N	2.34	0.43
1:F:310:PRO:HB3	1:F:316:GLU:HA	2.00	0.43
1:G:29:TYR:OH	1:G:33:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ARG:NH2	1:A:53:ARG:NH1	2.67	0.43
1:A:487:ILE:HG12	1:A:531:LYS:NZ	2.34	0.43
1:B:117:ARG:HD2	1:B:117:ARG:HA	1.73	0.43
1:B:527:GLU:OE1	1:B:527:GLU:N	2.51	0.43
1:C:135:TYR:CZ	1:C:139:ARG:HD2	2.52	0.43
1:D:302:LEU:HD23	1:D:337:PHE:HE1	1.77	0.43
1:D:374:LEU:HD13	1:D:378:LEU:HG	1.99	0.43
1:F:299:TYR:HD2	1:F:309:MET:SD	2.41	0.43
1:F:310:PRO:HB3	1:F:316:GLU:HB3	2.00	0.43
1:H:35:ILE:O	1:H:36:PHE:HD1	2.01	0.43
1:A:163:SER:O	1:A:330:PRO:HG2	2.18	0.43
1:A:374:LEU:HD13	1:A:378:LEU:HG	1.99	0.43
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.71	0.43
1:B:154:PHE:HB2	1:B:285:CYS:SG	2.58	0.43
1:B:240:ILE:HG13	1:B:241:ASP:OD1	2.19	0.43
1:B:336:PHE:CZ	1:B:348:MET:HG2	2.54	0.43
1:C:24:ARG:NH2	1:C:53:ARG:NH1	2.67	0.43
1:C:129:THR:HA	1:C:132:ILE:HD11	2.00	0.43
1:C:452:LEU:HD23	1:C:452:LEU:N	2.28	0.43
1:D:477:ILE:O	1:D:481:GLU:HG3	2.19	0.43
1:E:116:ASP:N	1:E:116:ASP:OD1	2.49	0.43
1:F:248:VAL:HG22	1:F:269:LEU:HD12	1.99	0.43
1:A:101:LEU:CD1	1:A:105:VAL:HB	2.47	0.43
1:A:307:MET:HA	1:A:308:PRO:HD3	1.82	0.43
1:A:527:GLU:N	1:A:527:GLU:OE1	2.51	0.43
1:B:388:GLU:H	1:B:388:GLU:HG3	1.60	0.43
1:B:479:ILE:HG23	1:B:483:ARG:CZ	2.48	0.43
1:C:388:GLU:O	1:C:391:SER:HB3	2.19	0.43
1:C:484:LEU:O	1:C:486:GLU:HG2	2.19	0.43
1:D:273:ARG:NH2	1:D:380:ARG:HH21	2.16	0.43
1:E:397:VAL:HG11	1:E:465:LYS:HA	2.01	0.43
1:E:414:ILE:HG21	1:E:430:VAL:HG13	2.01	0.43
1:F:128:MET:HA	1:F:128:MET:HE2	2.00	0.43
1:F:444:LEU:HD12	1:F:444:LEU:HA	1.71	0.43
1:H:8:ARG:NH1	1:H:8:ARG:CG	2.75	0.43
1:I:21:PHE:CG	1:I:22:GLU:N	2.87	0.43
1:A:273:ARG:NH2	1:A:380:ARG:HH21	2.16	0.43
1:C:67:GLU:HG2	1:C:68:LEU:N	2.33	0.43
1:C:540:TYR:O	1:C:543:LEU:HD23	2.18	0.43
1:E:340:CYS:HB3	1:E:343:LYS:HA	2.00	0.43
1:G:2:LEU:O	1:G:3:CYS:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:O	1:A:391:SER:HB3	2.19	0.43
1:A:414:ILE:HG21	1:A:430:VAL:HG13	2.01	0.43
1:B:24:ARG:NH2	1:B:53:ARG:NH1	2.67	0.43
1:B:165:LYS:HE3	1:B:272:THR:O	2.19	0.43
1:B:414:ILE:HG21	1:B:430:VAL:HG13	2.01	0.43
1:C:414:ILE:HG21	1:C:430:VAL:HG13	2.01	0.43
1:C:484:LEU:HD13	1:C:533:MET:HG2	1.99	0.43
1:C:526:PRO:CB	1:C:529:PHE:HD2	2.31	0.43
1:E:342:PRO:CG	1:E:347:LYS:HG3	2.49	0.43
1:F:307:MET:HA	1:F:308:PRO:HD3	1.82	0.43
1:H:35:ILE:HG22	1:H:36:PHE:CD1	2.54	0.43
1:A:154:PHE:HE2	1:A:262:GLN:HG3	1.83	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.78	0.43
1:B:111:SER:O	1:B:114:MET:HB2	2.18	0.43
1:B:228:SER:O	1:B:232:LYS:HG3	2.18	0.43
1:C:233:ARG:NH2	1:E:214:GLU:OE2	2.52	0.43
1:D:388:GLU:O	1:D:391:SER:HB3	2.19	0.43
1:F:273:ARG:NH2	1:F:380:ARG:HH21	2.16	0.43
1:F:321:LYS:O	1:F:325:LEU:HG	2.18	0.43
1:I:72:ILE:HG21	1:I:88:GLU:CG	2.46	0.43
1:A:302:LEU:CD2	1:A:337:PHE:HE1	2.31	0.43
1:B:273:ARG:NH2	1:B:380:ARG:HH21	2.16	0.43
1:C:8:ARG:HA	1:C:243:PRO:CG	2.49	0.43
1:C:165:LYS:HE3	1:C:272:THR:O	2.19	0.43
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.79	0.43
1:C:342:PRO:O	1:C:343:LYS:HB3	2.17	0.43
1:D:456:ILE:HD13	1:D:461:HIS:CD2	2.54	0.43
1:E:165:LYS:HE3	1:E:272:THR:O	2.19	0.43
1:E:235:ILE:O	1:E:239:LEU:N	2.52	0.43
1:G:21:PHE:CG	1:G:22:GLU:N	2.87	0.43
1:G:35:ILE:O	1:G:36:PHE:HD1	2.01	0.43
1:I:8:ARG:NH1	1:I:8:ARG:CG	2.75	0.43
1:A:175:LYS:NZ	1:A:175:LYS:HB3	2.33	0.42
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.52	0.42
1:D:315:GLU:HB3	1:D:345:PHE:CZ	2.54	0.42
1:E:274:ASP:O	1:E:277:ILE:HG12	2.18	0.42
1:B:8:ARG:NH1	1:B:8:ARG:CG	2.74	0.42
1:C:68:LEU:HD13	1:C:72:ILE:HG12	2.01	0.42
1:C:184:TYR:HA	1:C:244:ASN:HB3	2.02	0.42
1:D:165:LYS:HE3	1:D:272:THR:O	2.19	0.42
1:D:240:ILE:HG13	1:D:241:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ILE:HG21	1:D:430:VAL:HG13	2.01	0.42
1:D:484:LEU:O	1:D:531:LYS:HA	2.19	0.42
1:A:123:ASN:HD22	1:A:123:ASN:HA	1.63	0.42
1:B:391:SER:O	1:B:395:PHE:HD2	2.02	0.42
1:C:86:PHE:HE2	1:C:109:GLN:HE21	1.65	0.42
1:D:233:ARG:CG	1:D:233:ARG:NH1	2.80	0.42
1:E:329:ASN:HD22	1:E:330:PRO:HD2	1.84	0.42
1:E:405:ILE:HA	1:E:406:PRO:HD3	1.82	0.42
1:F:330:PRO:HB2	3:F:602:ATP:C8	2.54	0.42
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.85	0.42
1:C:1:MET:SD	1:C:2:LEU:N	2.92	0.42
1:C:106:ILE:CG2	1:C:182:ILE:HA	2.49	0.42
1:C:143:LYS:O	1:C:147:MET:HE3	2.20	0.42
1:C:366:ILE:H	1:C:366:ILE:CD1	2.20	0.42
1:D:204:PHE:CD2	1:D:207:ILE:HD12	2.54	0.42
1:E:269:LEU:HD22	1:E:270:VAL:N	2.34	0.42
1:E:484:LEU:HD21	1:E:533:MET:CG	2.49	0.42
1:G:35:ILE:HG22	1:G:36:PHE:CD1	2.54	0.42
1:I:35:ILE:HG22	1:I:36:PHE:CD1	2.54	0.42
1:C:342:PRO:C	1:C:344:THR:H	2.23	0.42
1:D:313:GLU:O	1:D:316:GLU:HG3	2.18	0.42
1:E:397:VAL:HG22	1:E:464:LEU:HB3	2.01	0.42
1:A:269:LEU:HD22	1:A:270:VAL:N	2.34	0.42
1:A:321:LYS:O	1:A:325:LEU:HG	2.20	0.42
1:B:100:LEU:HG	1:B:104:VAL:HG21	2.02	0.42
1:B:121:LEU:HA	1:D:233:ARG:HD3	2.01	0.42
1:B:534:GLN:NE2	1:B:534:GLN:CA	2.80	0.42
1:C:162:GLY:C	1:C:164:GLY:H	2.22	0.42
1:E:154:PHE:HE2	1:E:262:GLN:HG3	1.83	0.42
1:F:410:TRP:CZ3	1:F:454:PHE:HB2	2.55	0.42
1:F:414:ILE:HG21	1:F:430:VAL:HG13	2.01	0.42
1:A:127:GLN:OE1	1:A:171:GLN:HG2	2.20	0.42
1:A:302:LEU:CD2	1:A:337:PHE:CE1	3.01	0.42
1:A:366:ILE:H	1:A:366:ILE:CD1	2.20	0.42
1:A:400:PRO:HA	1:A:401:PRO:HD3	1.91	0.42
1:B:72:ILE:HG23	1:B:84:ALA:HB1	2.01	0.42
1:B:128:MET:HE1	1:D:282:SER:HB2	2.00	0.42
1:B:187:ILE:HD12	1:B:246:LEU:O	2.20	0.42
1:B:255:GLU:HB3	1:B:277:ILE:HG22	2.02	0.42
1:E:394:ALA:O	1:E:397:VAL:HG23	2.20	0.42
1:E:407:VAL:HG21	1:E:452:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:PHE:CG	1:H:22:GLU:N	2.87	0.42
1:A:391:SER:O	1:A:395:PHE:HD2	2.02	0.42
1:B:117:ARG:HH22	1:D:240:ILE:HA	1.85	0.42
1:B:434:LEU:HB3	1:B:444:LEU:CD2	2.50	0.42
1:E:126:LYS:HB3	1:E:126:LYS:HE2	1.84	0.42
1:E:313:GLU:O	1:E:316:GLU:HG3	2.18	0.42
1:F:426:LEU:HA	1:F:426:LEU:HD23	1.75	0.42
1:A:385:LEU:HD11	1:A:393:LEU:HD12	2.02	0.42
1:A:532:PHE:C	1:A:534:GLN:N	2.70	0.42
1:B:4:GLU:HG3	1:B:5:ILE:H	1.84	0.42
1:C:178:GLN:O	1:C:182:ILE:HB	2.20	0.42
1:C:233:ARG:HH11	1:C:237:ASN:HD21	1.68	0.42
1:C:283:GLN:HG3	1:E:126:LYS:HZ3	1.84	0.42
1:C:456:ILE:HD11	1:C:461:HIS:HA	2.01	0.42
1:D:269:LEU:HD22	1:D:270:VAL:N	2.34	0.42
1:D:407:VAL:HG21	1:D:452:LEU:HD12	2.02	0.42
1:E:187:ILE:HD13	1:E:246:LEU:HB3	2.02	0.42
1:E:211:LEU:HD13	1:E:238:ALA:HB3	2.02	0.42
1:F:269:LEU:HD22	1:F:270:VAL:N	2.35	0.42
1:A:126:LYS:HG2	1:A:127:GLN:N	2.35	0.42
1:A:397:VAL:HG22	1:A:464:LEU:CB	2.49	0.42
1:A:407:VAL:HG21	1:A:452:LEU:HD12	2.02	0.42
1:B:206:ASP:HA	1:B:209:LEU:HD12	2.02	0.42
1:C:24:ARG:CZ	1:C:53:ARG:HH11	2.33	0.42
1:C:123:ASN:HD22	1:C:123:ASN:HA	1.63	0.42
1:D:525:ARG:HA	1:D:526:PRO:HD3	1.70	0.42
1:E:347:LYS:HZ2	1:E:351:LEU:HD21	1.85	0.42
1:F:165:LYS:HE3	1:F:272:THR:O	2.19	0.42
1:G:72:ILE:HG23	1:G:84:ALA:HB1	2.01	0.42
1:A:165:LYS:HE3	1:A:272:THR:O	2.19	0.41
1:A:379:GLN:O	1:A:383:GLU:HG3	2.20	0.41
1:A:467:VAL:HG12	1:A:468:VAL:N	2.35	0.41
1:C:310:PRO:HA	1:C:345:PHE:HZ	1.83	0.41
1:D:190:LEU:HD23	1:D:190:LEU:HA	1.79	0.41
1:D:211:LEU:HD11	1:D:235:ILE:HG23	2.02	0.41
1:D:347:LYS:CE	1:D:351:LEU:HD21	2.50	0.41
1:E:130:CYS:O	1:E:304:ALA:HB1	2.20	0.41
1:E:391:SER:O	1:E:395:PHE:HD2	2.02	0.41
1:F:190:LEU:HD23	1:F:190:LEU:HA	1.79	0.41
1:F:283:GLN:CG	1:F:284:THR:H	2.29	0.41
1:F:366:ILE:H	1:F:366:ILE:CD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:67:GLU:HG2	1:I:69:GLY:H	1.85	0.41
1:A:24:ARG:CZ	1:A:53:ARG:HH11	2.33	0.41
1:A:233:ARG:CZ	1:A:237:ASN:HD21	2.33	0.41
1:B:1:MET:CE	1:F:117:ARG:NH2	2.83	0.41
1:B:3:CYS:O	1:B:4:GLU:C	2.59	0.41
1:B:112:ARG:O	1:B:115:LEU:HB2	2.20	0.41
1:B:130:CYS:O	1:B:304:ALA:HB1	2.20	0.41
1:B:204:PHE:CD2	1:B:207:ILE:HD12	2.55	0.41
1:C:160:ARG:HG2	1:C:161:ALA:H	1.84	0.41
1:D:388:GLU:H	1:D:388:GLU:HG3	1.60	0.41
1:D:434:LEU:HB3	1:D:444:LEU:CD2	2.50	0.41
1:E:115:LEU:HA	1:E:115:LEU:HD23	1.53	0.41
1:F:130:CYS:O	1:F:304:ALA:HB1	2.20	0.41
1:F:200:THR:HG21	1:F:256:GLU:HB3	2.02	0.41
1:F:394:ALA:O	1:F:397:VAL:HG23	2.20	0.41
1:A:178:GLN:O	1:A:182:ILE:HB	2.19	0.41
1:B:67:GLU:HG2	1:B:69:GLY:N	2.36	0.41
1:B:233:ARG:NH1	1:F:214:GLU:OE2	2.53	0.41
1:C:269:LEU:HD22	1:C:270:VAL:N	2.34	0.41
1:C:395:PHE:CG	1:C:413:VAL:O	2.73	0.41
1:C:406:PRO:CA	1:C:453:THR:HG22	2.47	0.41
1:D:468:VAL:O	1:D:469:ASP:C	2.59	0.41
1:E:521:GLU:C	1:E:523:VAL:N	2.74	0.41
1:G:46:LYS:HG3	1:G:46:LYS:H	1.76	0.41
1:I:35:ILE:O	1:I:36:PHE:CD1	2.74	0.41
1:A:239:LEU:HD22	1:A:242:ARG:HB2	2.03	0.41
1:B:379:GLN:O	1:B:383:GLU:HG3	2.20	0.41
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.75	0.41
1:C:1:MET:CE	1:C:240:ILE:HB	2.51	0.41
1:C:32:GLY:O	1:C:34:ASN:N	2.54	0.41
1:C:240:ILE:CG1	1:C:241:ASP:OD1	2.68	0.41
1:C:343:LYS:HD2	1:C:343:LYS:C	2.41	0.41
1:C:391:SER:O	1:C:393:LEU:N	2.52	0.41
1:C:444:LEU:HG	1:C:454:PHE:HB3	2.02	0.41
1:C:459:ILE:HG13	1:C:460:ILE:H	1.85	0.41
1:D:160:ARG:HH11	1:D:460:ILE:HD13	1.85	0.41
1:D:164:GLY:HA2	3:D:602:ATP:O1A	2.21	0.41
1:D:385:LEU:HD11	1:D:393:LEU:HD12	2.02	0.41
1:E:532:PHE:C	1:E:534:GLN:N	2.70	0.41
1:F:379:GLN:O	1:F:383:GLU:HG3	2.20	0.41
1:H:35:ILE:O	1:H:36:PHE:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:HG2	1:H:68:LEU:N	2.36	0.41
1:A:211:LEU:HA	1:A:242:ARG:NH2	2.36	0.41
1:A:487:ILE:HD13	1:A:487:ILE:N	2.35	0.41
1:A:521:GLU:C	1:A:523:VAL:N	2.74	0.41
1:C:8:ARG:NH1	1:C:8:ARG:CG	2.74	0.41
1:C:478:SER:O	1:C:482:GLN:HG2	2.21	0.41
1:D:206:ASP:HA	1:D:209:LEU:HD12	2.02	0.41
1:D:479:ILE:HG23	1:D:483:ARG:NH2	2.35	0.41
1:E:160:ARG:HG2	1:E:161:ALA:N	2.35	0.41
1:E:379:GLN:O	1:E:383:GLU:HG3	2.20	0.41
1:F:185:ASP:HB2	1:F:243:PRO:O	2.20	0.41
1:F:258:ILE:HD12	1:F:258:ILE:N	2.36	0.41
1:C:162:GLY:C	1:C:164:GLY:N	2.72	0.41
1:C:347:LYS:CE	1:C:351:LEU:HD21	2.50	0.41
1:D:182:ILE:N	1:D:182:ILE:CD1	2.84	0.41
1:D:379:GLN:O	1:D:383:GLU:HG3	2.20	0.41
1:E:162:GLY:C	1:E:164:GLY:N	2.73	0.41
1:E:319:LEU:O	1:E:323:ILE:HG13	2.20	0.41
1:E:329:ASN:HA	1:E:330:PRO:HD2	1.95	0.41
1:F:342:PRO:O	1:F:344:THR:N	2.54	0.41
1:F:369:TYR:C	1:F:371:TYR:H	2.24	0.41
1:I:24:ARG:NH2	1:I:53:ARG:NH1	2.69	0.41
1:A:26:ALA:HB2	1:A:74:PHE:CZ	2.56	0.41
1:A:175:LYS:HZ2	1:A:175:LYS:HB3	1.86	0.41
1:B:182:ILE:N	1:B:182:ILE:CD1	2.84	0.41
1:B:457:ASP:O	1:B:461:HIS:HB2	2.21	0.41
1:D:127:GLN:NE2	1:D:171:GLN:HG2	2.36	0.41
1:D:343:LYS:HE3	1:D:343:LYS:HB3	1.83	0.41
1:E:178:GLN:HA	1:E:182:ILE:HD13	2.02	0.41
1:F:343:LYS:HB3	1:F:343:LYS:HE3	1.78	0.41
1:H:24:ARG:NH2	1:H:53:ARG:NH1	2.69	0.41
1:H:67:GLU:HG2	1:H:69:GLY:H	1.85	0.41
1:A:255:GLU:O	1:A:259:ARG:HG3	2.20	0.41
1:A:457:ASP:OD1	1:A:457:ASP:N	2.54	0.41
1:B:269:LEU:HD22	1:B:270:VAL:N	2.34	0.41
1:B:334:MET:HG3	1:B:338:LYS:HE2	2.02	0.41
1:B:385:LEU:HD23	1:B:385:LEU:HA	1.85	0.41
1:C:240:ILE:CG1	1:C:241:ASP:N	2.83	0.41
1:C:312:GLY:O	1:C:315:GLU:HB2	2.20	0.41
1:D:185:ASP:HB2	1:D:243:PRO:O	2.21	0.41
1:D:316:GLU:OE1	1:D:320:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ILE:O	1:E:327:SER:N	2.53	0.41
1:F:207:ILE:O	1:F:211:LEU:HG	2.20	0.41
1:F:484:LEU:HG	1:F:531:LYS:O	2.21	0.41
1:A:481:GLU:O	1:A:484:LEU:HB2	2.20	0.41
1:B:24:ARG:CZ	1:B:53:ARG:HH11	2.33	0.41
1:B:344:THR:O	1:B:345:PHE:C	2.58	0.41
1:B:393:LEU:C	1:B:393:LEU:CD2	2.84	0.41
1:B:457:ASP:OD1	1:B:457:ASP:N	2.54	0.41
1:C:233:ARG:CG	1:C:233:ARG:NH1	2.80	0.41
1:C:379:GLN:O	1:C:383:GLU:HG3	2.20	0.41
1:C:407:VAL:HG21	1:C:452:LEU:HD12	2.02	0.41
1:D:184:TYR:HB3	1:D:244:ASN:O	2.21	0.41
1:D:456:ILE:CG1	1:D:460:ILE:CG2	2.92	0.41
1:F:240:ILE:CG1	1:F:241:ASP:N	2.83	0.41
1:F:310:PRO:CA	1:F:345:PHE:HZ	2.29	0.41
1:F:347:LYS:CE	1:F:351:LEU:HD21	2.50	0.41
1:G:67:GLU:HG2	1:G:68:LEU:N	2.36	0.41
1:H:22:GLU:OE1	1:H:50:ARG:HD2	2.21	0.41
1:H:72:ILE:HG23	1:H:84:ALA:HB1	2.02	0.41
1:I:22:GLU:OE1	1:I:50:ARG:HD2	2.21	0.41
1:A:347:LYS:CE	1:A:351:LEU:HD21	2.50	0.41
1:B:161:ALA:HA	1:B:273:ARG:HD3	2.03	0.41
1:B:347:LYS:CE	1:B:351:LEU:HD21	2.50	0.41
1:C:100:LEU:HG	1:C:104:VAL:HG21	2.02	0.41
1:C:457:ASP:OD1	1:C:457:ASP:N	2.54	0.41
1:C:467:VAL:HG12	1:C:468:VAL:N	2.35	0.41
1:D:385:LEU:HD23	1:D:385:LEU:HA	1.85	0.41
1:D:391:SER:O	1:D:395:PHE:HD2	2.04	0.41
1:D:457:ASP:N	1:D:457:ASP:OD1	2.54	0.41
1:D:521:GLU:C	1:D:523:VAL:N	2.74	0.41
1:E:369:TYR:C	1:E:371:TYR:H	2.24	0.41
1:E:426:LEU:HD23	1:E:426:LEU:HA	1.75	0.41
1:F:407:VAL:HG21	1:F:452:LEU:HD12	2.02	0.41
1:G:35:ILE:O	1:G:36:PHE:CD1	2.73	0.41
1:A:461:HIS:C	1:A:463:PHE:N	2.74	0.40
1:A:533:MET:C	1:A:533:MET:HE2	2.41	0.40
1:B:30:LEU:CD2	1:B:35:ILE:HD12	2.46	0.40
1:B:334:MET:CE	1:B:337:PHE:HD2	2.33	0.40
1:B:462:MET:HA	1:B:465:LYS:HB3	2.03	0.40
1:C:136:HIS:HB3	1:C:168:ILE:CD1	2.51	0.40
1:C:369:TYR:C	1:C:371:TYR:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ARG:HD2	1:F:117:ARG:HA	1.73	0.40
1:F:302:LEU:CD2	1:F:337:PHE:CE1	3.01	0.40
1:F:533:MET:C	1:F:533:MET:HE2	2.41	0.40
1:A:182:ILE:N	1:A:182:ILE:CD1	2.84	0.40
1:A:526:PRO:HG2	1:A:529:PHE:CD2	2.57	0.40
1:B:43:LEU:HD13	1:B:43:LEU:HA	1.96	0.40
1:B:204:PHE:C	1:B:231:LEU:HD21	2.42	0.40
1:B:397:VAL:HG22	1:B:464:LEU:HB3	2.03	0.40
1:C:302:LEU:CD2	1:C:337:PHE:CE1	3.01	0.40
1:D:198:LYS:N	1:D:198:LYS:HD3	2.37	0.40
1:D:457:ASP:O	1:D:461:HIS:HB2	2.21	0.40
1:E:167:VAL:HG12	1:E:168:ILE:N	2.36	0.40
1:E:176:SER:CB	1:E:179:LEU:HD22	2.49	0.40
1:E:182:ILE:N	1:E:182:ILE:CD1	2.84	0.40
1:E:240:ILE:HG13	1:E:241:ASP:OD1	2.21	0.40
1:E:335:MET:CE	1:E:373:SER:HA	2.52	0.40
1:E:457:ASP:OD1	1:E:457:ASP:N	2.54	0.40
1:F:141:ILE:CD1	1:F:175:LYS:HZ2	2.34	0.40
1:F:155:LEU:HD23	1:F:286:GLU:HB2	2.02	0.40
1:G:24:ARG:NH2	1:G:53:ARG:NH1	2.69	0.40
1:H:64:GLN:HE21	1:H:64:GLN:CA	2.29	0.40
1:A:310:PRO:HB3	1:A:316:GLU:HA	2.02	0.40
1:A:369:TYR:C	1:A:371:TYR:H	2.24	0.40
1:B:369:TYR:C	1:B:371:TYR:H	2.24	0.40
1:C:309:MET:HG3	1:C:310:PRO:HD2	2.02	0.40
1:C:390:ARG:HE	1:C:390:ARG:HB2	1.61	0.40
1:D:302:LEU:CD2	1:D:337:PHE:CE1	3.01	0.40
1:D:335:MET:CE	1:D:373:SER:HA	2.52	0.40
1:D:447:LYS:HE2	1:D:449:MET:O	2.21	0.40
1:E:447:LYS:HE2	1:E:449:MET:O	2.20	0.40
1:A:136:HIS:HB3	1:A:168:ILE:CD1	2.51	0.40
1:A:153:PHE:CE1	1:A:267:ARG:HB3	2.57	0.40
1:A:234:MET:HE3	1:A:234:MET:HB2	1.97	0.40
1:A:395:PHE:O	1:A:398:VAL:HG22	2.21	0.40
1:B:200:THR:HG23	1:B:257:THR:HA	2.03	0.40
1:B:407:VAL:HG21	1:B:452:LEU:HD12	2.02	0.40
1:C:93:PHE:CD2	1:C:100:LEU:HB3	2.55	0.40
1:C:204:PHE:C	1:C:231:LEU:HD21	2.42	0.40
1:D:148:CYS:SG	1:D:183:ASN:ND2	2.94	0.40
1:D:344:THR:O	1:D:345:PHE:C	2.59	0.40
1:E:329:ASN:O	1:E:330:PRO:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ASP:OD2	1:F:243:PRO:HG2	2.21	0.40
1:F:335:MET:CE	1:F:373:SER:HA	2.52	0.40
1:F:354:LYS:O	1:F:358:ARG:HB2	2.22	0.40
1:F:526:PRO:HG2	1:F:529:PHE:CD2	2.57	0.40
1:I:24:ARG:CZ	1:I:53:ARG:HH11	2.35	0.40
1:A:204:PHE:C	1:A:231:LEU:HD21	2.42	0.40
1:B:167:VAL:HG12	1:B:168:ILE:N	2.37	0.40
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.78	0.40
1:C:212:LYS:HA	1:C:212:LYS:CE	2.30	0.40
1:D:153:PHE:CE1	1:D:267:ARG:HB3	2.57	0.40
1:E:354:LYS:O	1:E:358:ARG:HB2	2.22	0.40
1:E:526:PRO:HG2	1:E:529:PHE:CD2	2.56	0.40
1:F:203:LEU:HD11	1:F:249:PHE:CE1	2.57	0.40
1:F:310:PRO:HG3	1:F:316:GLU:HA	2.04	0.40
1:F:341:GLU:HB2	1:F:342:PRO:HD3	2.04	0.40
1:I:72:ILE:HG23	1:I:84:ALA:HB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/549 (90%)	417 (84%)	77 (16%)	3 (1%)	25	64
1	B	497/549 (90%)	438 (88%)	59 (12%)	0	100	100
1	C	497/549 (90%)	433 (87%)	63 (13%)	1 (0%)	47	80
1	D	386/549 (70%)	342 (89%)	42 (11%)	2 (0%)	29	68
1	E	386/549 (70%)	336 (87%)	46 (12%)	4 (1%)	15	54
1	F	386/549 (70%)	338 (88%)	44 (11%)	4 (1%)	15	54
1	G	98/549 (18%)	82 (84%)	14 (14%)	2 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	98/549 (18%)	78 (80%)	16 (16%)	4 (4%)	3	26
1	I	98/549 (18%)	78 (80%)	16 (16%)	4 (4%)	3	26
All	All	2943/4941 (60%)	2542 (86%)	377 (13%)	24 (1%)	24	60

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	212	LYS
1	F	445	SER
1	A	130	CYS
1	A	522	THR
1	D	522	THR
1	E	283	GLN
1	E	398	VAL
1	E	522	THR
1	F	522	THR
1	C	310	PRO
1	G	2	LEU
1	H	2	LEU
1	H	73	ASP
1	I	2	LEU
1	I	73	ASP
1	A	311	VAL
1	D	175	LYS
1	E	484	LEU
1	F	283	GLN
1	G	35	ILE
1	H	35	ILE
1	I	35	ILE
1	H	70	PRO
1	I	70	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/501 (91%)	377 (82%)	81 (18%)	2	12
1	B	458/501 (91%)	388 (85%)	70 (15%)	2	16
1	C	458/501 (91%)	390 (85%)	68 (15%)	3	17
1	D	357/501 (71%)	305 (85%)	52 (15%)	3	18
1	E	357/501 (71%)	301 (84%)	56 (16%)	2	16
1	F	357/501 (71%)	300 (84%)	57 (16%)	2	15
1	G	91/501 (18%)	78 (86%)	13 (14%)	3	18
1	H	91/501 (18%)	78 (86%)	13 (14%)	3	18
1	I	91/501 (18%)	78 (86%)	13 (14%)	3	18
All	All	2718/4509 (60%)	2295 (84%)	423 (16%)	5	16

All (423) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLU
1	A	15	THR
1	A	17	LEU
1	A	45	SER
1	A	46	LYS
1	A	51	LEU
1	A	52	GLU
1	A	64	GLN
1	A	67	GLU
1	A	68	LEU
1	A	71	LEU
1	A	73	ASP
1	A	77	TYR
1	A	95	ILE
1	A	117	ARG
1	A	131	TYR
1	A	148	CYS
1	A	155	LEU
1	A	157	LEU
1	A	160	ARG
1	A	174	SER
1	A	175	LYS
1	A	179	LEU
1	A	180	ILE
1	A	185	ASP

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Mol	Chain	Res	Type
1	A	189	TRP
1	A	198	LYS
1	A	203	LEU
1	A	208	LEU
1	A	217	LEU
1	A	218	LEU
1	A	220	PHE
1	A	223	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	253	VAL
1	A	255	GLU
1	A	262	GLN
1	A	269	LEU
1	A	277	ILE
1	A	286	GLU
1	A	296	ASP
1	A	309	MET
1	A	316	GLU
1	A	332	THR
1	A	341	GLU
1	A	343	LYS
1	A	344	THR
1	A	348	MET
1	A	355	LEU
1	A	360	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
1	A	381	CYS
1	A	382	VAL
1	A	387	ASP
1	A	404	ASP
1	A	405	ILE
1	A	408	LYS
1	A	409	LEU
1	A	410	TRP
1	A	437	LEU
1	A	444	LEU
1	A	451	VAL

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	465	LYS
1	A	466	HIS
1	A	484	LEU
1	A	485	LEU
1	A	487	ILE
1	A	525	ARG
1	A	533	MET
1	A	539	PHE
1	A	542	SER
1	A	543	LEU
1	B	1	MET
1	B	15	THR
1	B	17	LEU
1	B	45	SER
1	B	46	LYS
1	B	51	LEU
1	B	52	GLU
1	B	64	GLN
1	B	67	GLU
1	B	68	LEU
1	B	77	TYR
1	B	95	ILE
1	B	110	PHE
1	B	113	GLN
1	B	115	LEU
1	B	116	ASP
1	B	117	ARG
1	B	130	CYS
1	B	131	TYR
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	174	SER
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	217	LEU
1	B	218	LEU
1	B	220	PHE
1	B	223	VAL
1	B	227	THR
1	B	239	LEU
1	B	245	THR
1	B	253	VAL
1	B	269	LEU
1	B	277	ILE
1	B	296	ASP
1	B	309	MET
1	B	316	GLU
1	B	332	THR
1	B	338	LYS
1	B	348	MET
1	B	355	LEU
1	B	360	LEU
1	B	363	VAL
1	B	364	GLU
1	B	366	ILE
1	B	369	TYR
1	B	381	CYS
1	B	382	VAL
1	B	387	ASP
1	B	393	LEU
1	B	404	ASP
1	B	405	ILE
1	B	408	LYS
1	B	409	LEU
1	B	410	TRP
1	B	437	LEU
1	B	451	VAL
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	525	ARG
1	B	533	MET
1	B	539	PHE
1	B	542	SER
1	B	543	LEU
1	C	1	MET

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Mol	Chain	Res	Type
1	C	15	THR
1	C	17	LEU
1	C	45	SER
1	C	46	LYS
1	C	51	LEU
1	C	52	GLU
1	C	64	GLN
1	C	67	GLU
1	C	68	LEU
1	C	77	TYR
1	C	95	ILE
1	C	110	PHE
1	C	113	GLN
1	C	115	LEU
1	C	116	ASP
1	C	117	ARG
1	C	131	TYR
1	C	148	CYS
1	C	155	LEU
1	C	157	LEU
1	C	179	LEU
1	C	180	ILE
1	C	185	ASP
1	C	189	TRP
1	C	198	LYS
1	C	203	LEU
1	C	217	LEU
1	C	218	LEU
1	C	220	PHE
1	C	223	VAL
1	C	227	THR
1	C	233	ARG
1	C	239	LEU
1	C	241	ASP
1	C	253	VAL
1	C	269	LEU
1	C	277	ILE
1	C	296	ASP
1	C	309	MET
1	C	316	GLU
1	C	332	THR
1	C	343	LYS

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Mol	Chain	Res	Type
1	C	344	THR
1	C	348	MET
1	C	355	LEU
1	C	360	LEU
1	C	363	VAL
1	C	364	GLU
1	C	366	ILE
1	C	369	TYR
1	C	381	CYS
1	C	382	VAL
1	C	387	ASP
1	C	404	ASP
1	C	405	ILE
1	C	408	LYS
1	C	409	LEU
1	C	410	TRP
1	C	437	LEU
1	C	451	VAL
1	C	452	LEU
1	C	457	ASP
1	C	525	ARG
1	C	533	MET
1	C	539	PHE
1	C	542	SER
1	C	543	LEU
1	D	113	GLN
1	D	115	LEU
1	D	116	ASP
1	D	117	ARG
1	D	148	CYS
1	D	155	LEU
1	D	157	LEU
1	D	174	SER
1	D	179	LEU
1	D	180	ILE
1	D	185	ASP
1	D	189	TRP
1	D	198	LYS
1	D	203	LEU
1	D	217	LEU
1	D	218	LEU
1	D	220	PHE

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Mol	Chain	Res	Type
1	D	223	VAL
1	D	227	THR
1	D	233	ARG
1	D	262	GLN
1	D	269	LEU
1	D	277	ILE
1	D	296	ASP
1	D	309	MET
1	D	332	THR
1	D	343	LYS
1	D	348	MET
1	D	355	LEU
1	D	360	LEU
1	D	363	VAL
1	D	364	GLU
1	D	366	ILE
1	D	369	TYR
1	D	381	CYS
1	D	382	VAL
1	D	387	ASP
1	D	404	ASP
1	D	405	ILE
1	D	408	LYS
1	D	409	LEU
1	D	410	TRP
1	D	437	LEU
1	D	451	VAL
1	D	452	LEU
1	D	457	ASP
1	D	459	ILE
1	D	525	ARG
1	D	533	MET
1	D	539	PHE
1	D	542	SER
1	D	543	LEU
1	E	113	GLN
1	E	115	LEU
1	E	116	ASP
1	E	128	MET
1	E	130	CYS
1	E	131	TYR
1	E	148	CYS

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Mol	Chain	Res	Type
1	E	155	LEU
1	E	157	LEU
1	E	179	LEU
1	E	180	ILE
1	E	185	ASP
1	E	189	TRP
1	E	198	LYS
1	E	203	LEU
1	E	217	LEU
1	E	218	LEU
1	E	220	PHE
1	E	223	VAL
1	E	227	THR
1	E	236	CYS
1	E	239	LEU
1	E	255	GLU
1	E	262	GLN
1	E	269	LEU
1	E	277	ILE
1	E	296	ASP
1	E	329	ASN
1	E	332	THR
1	E	343	LYS
1	E	348	MET
1	E	355	LEU
1	E	360	LEU
1	E	363	VAL
1	E	364	GLU
1	E	366	ILE
1	E	369	TYR
1	E	381	CYS
1	E	382	VAL
1	E	387	ASP
1	E	404	ASP
1	E	405	ILE
1	E	408	LYS
1	E	409	LEU
1	E	410	TRP
1	E	437	LEU
1	E	451	VAL
1	E	452	LEU
1	E	457	ASP

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Mol	Chain	Res	Type
1	E	485	LEU
1	E	486	GLU
1	E	525	ARG
1	E	533	MET
1	E	539	PHE
1	E	542	SER
1	E	543	LEU
1	F	113	GLN
1	F	115	LEU
1	F	116	ASP
1	F	117	ARG
1	F	128	MET
1	F	130	CYS
1	F	131	TYR
1	F	148	CYS
1	F	155	LEU
1	F	157	LEU
1	F	179	LEU
1	F	180	ILE
1	F	185	ASP
1	F	189	TRP
1	F	198	LYS
1	F	217	LEU
1	F	218	LEU
1	F	220	PHE
1	F	223	VAL
1	F	227	THR
1	F	229	VAL
1	F	239	LEU
1	F	241	ASP
1	F	253	VAL
1	F	255	GLU
1	F	269	LEU
1	F	277	ILE
1	F	296	ASP
1	F	316	GLU
1	F	332	THR
1	F	341	GLU
1	F	343	LYS
1	F	344	THR
1	F	348	MET
1	F	355	LEU

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Mol	Chain	Res	Type
1	F	360	LEU
1	F	363	VAL
1	F	364	GLU
1	F	366	ILE
1	F	369	TYR
1	F	381	CYS
1	F	382	VAL
1	F	387	ASP
1	F	404	ASP
1	F	405	ILE
1	F	408	LYS
1	F	409	LEU
1	F	410	TRP
1	F	437	LEU
1	F	444	LEU
1	F	451	VAL
1	F	452	LEU
1	F	525	ARG
1	F	533	MET
1	F	539	PHE
1	F	542	SER
1	F	543	LEU
1	G	1	MET
1	G	4	GLU
1	G	15	THR
1	G	17	LEU
1	G	45	SER
1	G	46	LYS
1	G	52	GLU
1	G	64	GLN
1	G	67	GLU
1	G	68	LEU
1	G	77	TYR
1	G	97	GLU
1	G	99	ASP
1	H	1	MET
1	H	4	GLU
1	H	15	THR
1	H	17	LEU
1	H	45	SER
1	H	46	LYS
1	H	52	GLU

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Mol	Chain	Res	Type
1	H	64	GLN
1	H	67	GLU
1	H	68	LEU
1	H	77	TYR
1	H	97	GLU
1	H	99	ASP
1	I	1	MET
1	I	4	GLU
1	I	15	THR
1	I	17	LEU
1	I	45	SER
1	I	46	LYS
1	I	52	GLU
1	I	64	GLN
1	I	67	GLU
1	I	68	LEU
1	I	77	TYR
1	I	97	GLU
1	I	99	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	64	GLN
1	A	78	ASN
1	A	123	ASN
1	A	171	GLN
1	A	219	ASN
1	A	237	ASN
1	A	244	ASN
1	A	471	GLN
1	A	482	GLN
1	A	534	GLN
1	B	34	ASN
1	B	64	GLN
1	B	78	ASN
1	B	171	GLN
1	B	219	ASN
1	B	283	GLN
1	B	471	GLN
1	B	482	GLN

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Mol	Chain	Res	Type
1	B	534	GLN
1	C	34	ASN
1	C	64	GLN
1	C	78	ASN
1	C	219	ASN
1	C	262	GLN
1	C	471	GLN
1	C	482	GLN
1	C	534	GLN
1	D	123	ASN
1	D	219	ASN
1	D	244	ASN
1	D	262	GLN
1	D	283	GLN
1	D	471	GLN
1	D	482	GLN
1	D	534	GLN
1	E	123	ASN
1	E	219	ASN
1	E	244	ASN
1	E	283	GLN
1	E	461	HIS
1	E	471	GLN
1	E	534	GLN
1	F	123	ASN
1	F	219	ASN
1	F	244	ASN
1	F	283	GLN
1	F	461	HIS
1	F	471	GLN
1	F	482	GLN
1	F	534	GLN
1	G	34	ASN
1	G	40	HIS
1	G	78	ASN
1	H	34	ASN
1	H	40	HIS
1	H	78	ASN
1	I	34	ASN
1	I	40	HIS
1	I	78	ASN

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 ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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$
3	ATP	E	602	2	26,33,33	1.11	2 (7%)	31,52,52	1.91	10 (32%)
3	ATP	F	602	2	26,33,33	1.11	2 (7%)	31,52,52	1.91	10 (32%)
3	ATP	B	602	2	26,33,33	1.11	2 (7%)	31,52,52	1.92	10 (32%)
3	ATP	A	602	2	26,33,33	1.11	2 (7%)	31,52,52	1.91	10 (32%)
3	ATP	D	602	2	26,33,33	1.12	3 (11%)	31,52,52	1.91	10 (32%)
3	ATP	C	602	2	26,33,33	1.12	2 (7%)	31,52,52	1.91	10 (32%)

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
3	ATP	E	602	2	-	5/18/38/38	0/3/3/3
3	ATP	F	602	2	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	602	2	-	5/18/38/38	0/3/3/3
3	ATP	A	602	2	-	5/18/38/38	0/3/3/3
3	ATP	D	602	2	-	5/18/38/38	0/3/3/3
3	ATP	C	602	2	-	5/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	ATP	C5-C4	3.00	1.48	1.40
3	A	602	ATP	C5-C4	2.97	1.48	1.40
3	B	602	ATP	C5-C4	2.97	1.48	1.40
3	D	602	ATP	C5-C4	2.96	1.48	1.40
3	E	602	ATP	C5-C4	2.96	1.48	1.40
3	F	602	ATP	C5-C4	2.95	1.48	1.40
3	C	602	ATP	O4'-C1'	2.91	1.45	1.41
3	F	602	ATP	O4'-C1'	2.89	1.45	1.41
3	D	602	ATP	O4'-C1'	2.88	1.45	1.41
3	B	602	ATP	O4'-C1'	2.88	1.45	1.41
3	E	602	ATP	O4'-C1'	2.88	1.45	1.41
3	A	602	ATP	O4'-C1'	2.87	1.45	1.41
3	D	602	ATP	C2-N3	2.01	1.35	1.32

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ATP	PB-O3B-PG	-5.45	114.11	132.83
3	C	602	ATP	PB-O3B-PG	-5.45	114.13	132.83
3	A	602	ATP	PB-O3B-PG	-5.44	114.15	132.83
3	D	602	ATP	PB-O3B-PG	-5.44	114.16	132.83
3	E	602	ATP	PB-O3B-PG	-5.44	114.17	132.83
3	F	602	ATP	PB-O3B-PG	-5.43	114.19	132.83
3	A	602	ATP	C3'-C2'-C1'	3.73	106.59	100.98
3	C	602	ATP	C3'-C2'-C1'	3.72	106.57	100.98
3	F	602	ATP	C3'-C2'-C1'	3.70	106.54	100.98
3	B	602	ATP	C3'-C2'-C1'	3.70	106.54	100.98
3	D	602	ATP	C3'-C2'-C1'	3.70	106.54	100.98
3	E	602	ATP	C3'-C2'-C1'	3.69	106.54	100.98
3	B	602	ATP	PA-O3A-PB	-3.25	121.66	132.83
3	A	602	ATP	PA-O3A-PB	-3.25	121.67	132.83
3	F	602	ATP	PA-O3A-PB	-3.25	121.67	132.83
3	C	602	ATP	PA-O3A-PB	-3.25	121.68	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	602	ATP	PA-O3A-PB	-3.25	121.69	132.83
3	D	602	ATP	PA-O3A-PB	-3.24	121.71	132.83
3	D	602	ATP	O3G-PG-O2G	2.69	117.92	107.64
3	B	602	ATP	O3G-PG-O2G	2.69	117.92	107.64
3	A	602	ATP	O3G-PG-O2G	2.69	117.91	107.64
3	C	602	ATP	O3G-PG-O2G	2.69	117.90	107.64
3	F	602	ATP	O3G-PG-O2G	2.69	117.90	107.64
3	E	602	ATP	O3G-PG-O2G	2.68	117.89	107.64
3	B	602	ATP	N3-C2-N1	-2.61	124.60	128.68
3	D	602	ATP	N3-C2-N1	-2.60	124.61	128.68
3	E	602	ATP	N3-C2-N1	-2.60	124.62	128.68
3	C	602	ATP	N3-C2-N1	-2.58	124.64	128.68
3	F	602	ATP	N3-C2-N1	-2.55	124.69	128.68
3	A	602	ATP	N3-C2-N1	-2.55	124.70	128.68
3	B	602	ATP	O2B-PB-O1B	2.45	124.34	112.24
3	A	602	ATP	O2B-PB-O1B	2.45	124.34	112.24
3	E	602	ATP	O2B-PB-O1B	2.44	124.32	112.24
3	F	602	ATP	O2B-PB-O1B	2.44	124.30	112.24
3	D	602	ATP	O2B-PB-O1B	2.44	124.30	112.24
3	C	602	ATP	O2B-PB-O1B	2.44	124.29	112.24
3	A	602	ATP	O3G-PG-O3B	-2.35	96.76	104.64
3	B	602	ATP	O3G-PG-O3B	-2.34	96.78	104.64
3	C	602	ATP	O3G-PG-O3B	-2.34	96.78	104.64
3	D	602	ATP	O3G-PG-O3B	-2.34	96.79	104.64
3	F	602	ATP	O3G-PG-O3B	-2.33	96.83	104.64
3	E	602	ATP	O3G-PG-O3B	-2.32	96.84	104.64
3	D	602	ATP	C4-C5-N7	-2.11	107.20	109.40
3	C	602	ATP	C4-C5-N7	-2.11	107.20	109.40
3	F	602	ATP	C4-C5-N7	-2.11	107.20	109.40
3	A	602	ATP	C4-C5-N7	-2.10	107.21	109.40
3	B	602	ATP	C4-C5-N7	-2.10	107.21	109.40
3	E	602	ATP	C4-C5-N7	-2.09	107.22	109.40
3	D	602	ATP	O2'-C2'-C3'	-2.05	105.19	111.82
3	E	602	ATP	O2'-C2'-C3'	-2.05	105.19	111.82
3	A	602	ATP	O2'-C2'-C3'	-2.05	105.19	111.82
3	C	602	ATP	O2'-C2'-C3'	-2.05	105.20	111.82
3	F	602	ATP	O2'-C2'-C3'	-2.04	105.22	111.82
3	F	602	ATP	O5'-C5'-C4'	-2.04	101.98	108.99
3	B	602	ATP	O2'-C2'-C3'	-2.03	105.24	111.82
3	E	602	ATP	O5'-C5'-C4'	-2.03	101.99	108.99
3	C	602	ATP	O5'-C5'-C4'	-2.03	102.00	108.99
3	A	602	ATP	O5'-C5'-C4'	-2.03	102.01	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ATP	O5'-C5'-C4'	-2.03	102.01	108.99
3	D	602	ATP	O5'-C5'-C4'	-2.01	102.07	108.99

There are no chirality outliers.

All (30) torsion outliers are listed below:

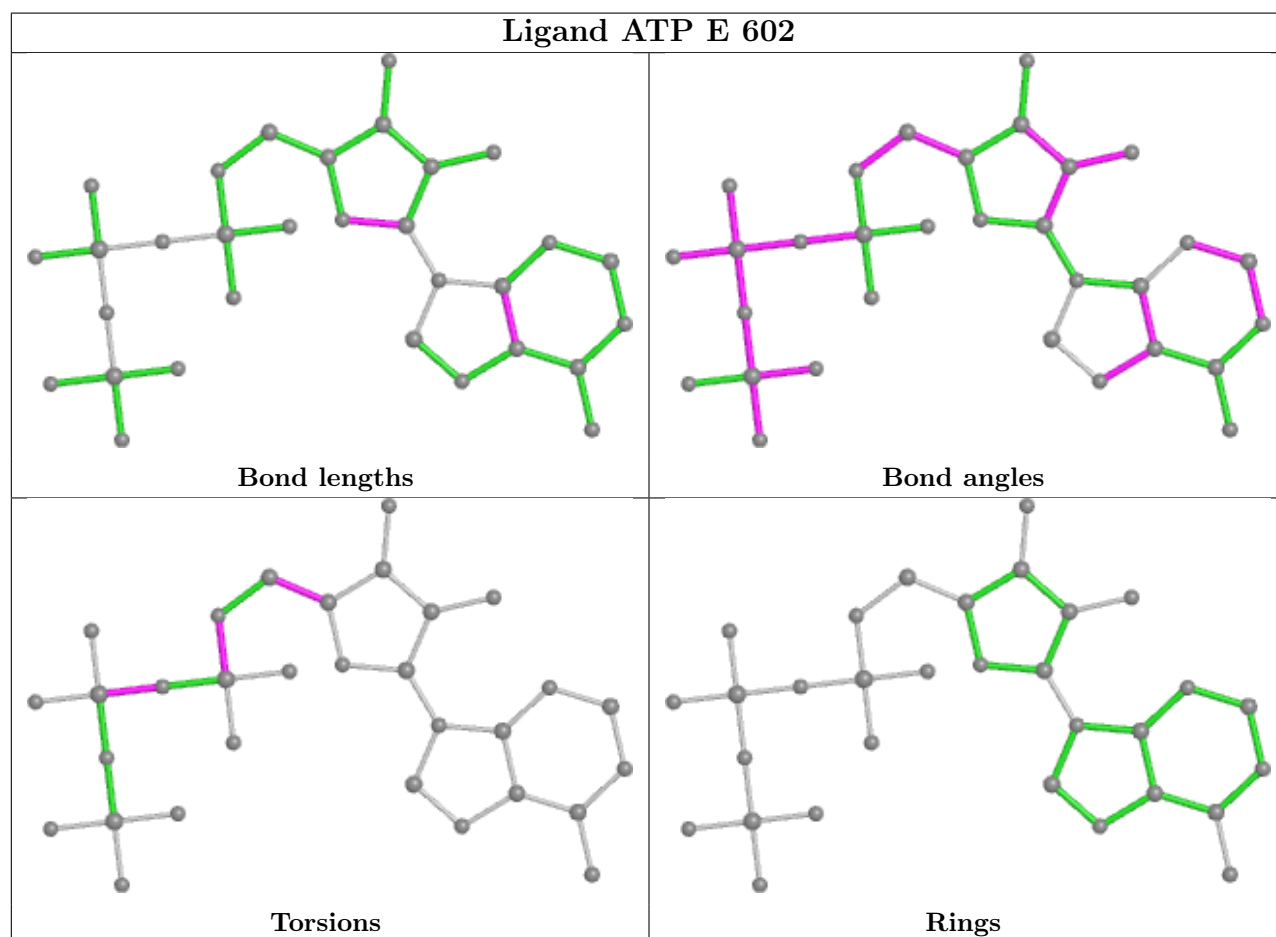
Mol	Chain	Res	Type	Atoms
3	A	602	ATP	C5'-O5'-PA-O3A
3	A	602	ATP	O4'-C4'-C5'-O5'
3	A	602	ATP	C3'-C4'-C5'-O5'
3	B	602	ATP	C5'-O5'-PA-O3A
3	B	602	ATP	O4'-C4'-C5'-O5'
3	B	602	ATP	C3'-C4'-C5'-O5'
3	C	602	ATP	C5'-O5'-PA-O3A
3	C	602	ATP	O4'-C4'-C5'-O5'
3	C	602	ATP	C3'-C4'-C5'-O5'
3	D	602	ATP	C5'-O5'-PA-O3A
3	D	602	ATP	O4'-C4'-C5'-O5'
3	D	602	ATP	C3'-C4'-C5'-O5'
3	E	602	ATP	C5'-O5'-PA-O3A
3	E	602	ATP	O4'-C4'-C5'-O5'
3	E	602	ATP	C3'-C4'-C5'-O5'
3	F	602	ATP	C5'-O5'-PA-O3A
3	F	602	ATP	O4'-C4'-C5'-O5'
3	F	602	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O1A
3	C	602	ATP	C5'-O5'-PA-O1A
3	D	602	ATP	C5'-O5'-PA-O1A
3	E	602	ATP	C5'-O5'-PA-O1A
3	F	602	ATP	C5'-O5'-PA-O1A
3	A	602	ATP	PA-O3A-PB-O1B
3	B	602	ATP	PA-O3A-PB-O1B
3	C	602	ATP	PA-O3A-PB-O1B
3	D	602	ATP	PA-O3A-PB-O1B
3	E	602	ATP	PA-O3A-PB-O1B
3	F	602	ATP	PA-O3A-PB-O1B

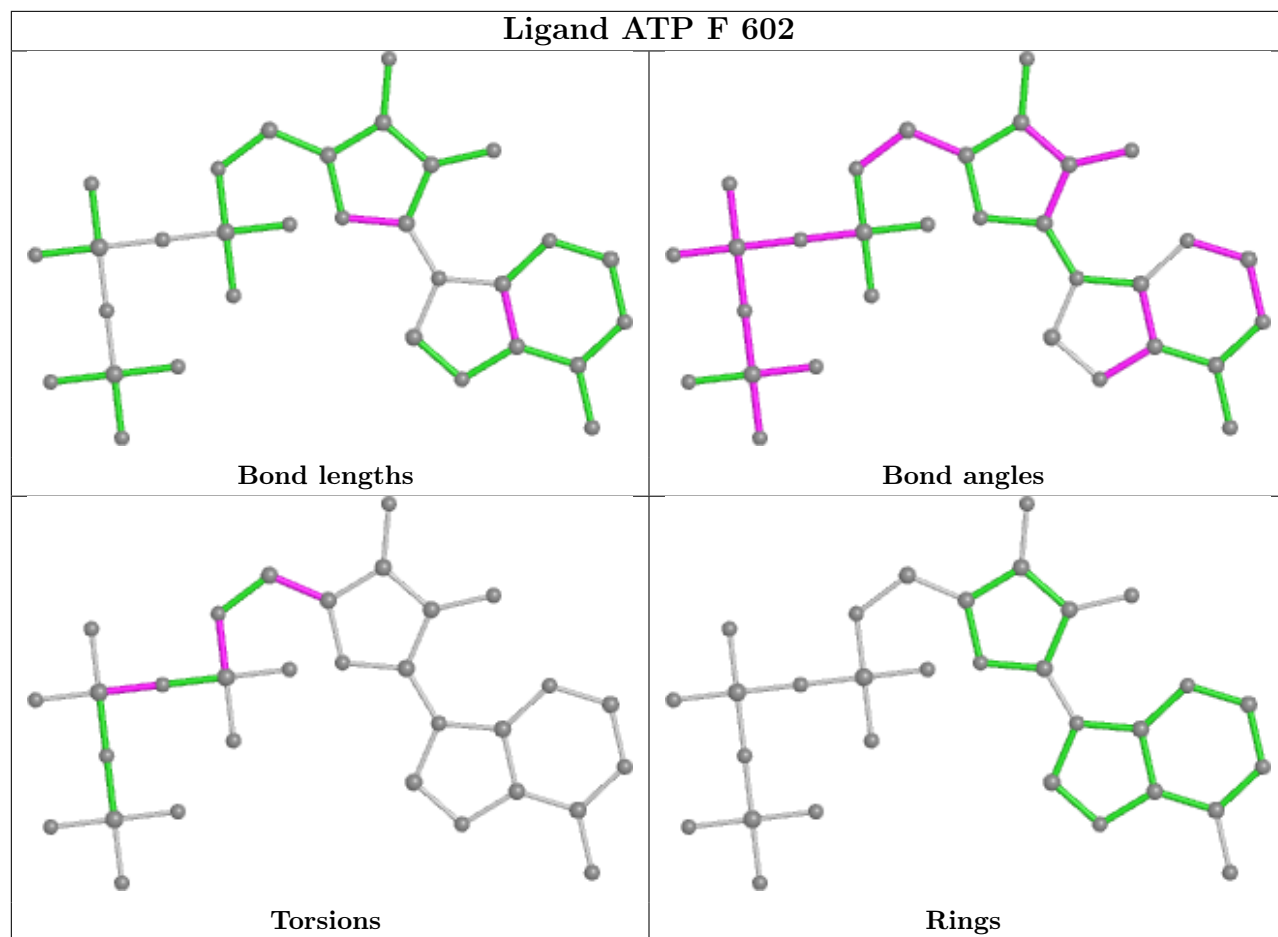
There are no ring outliers.

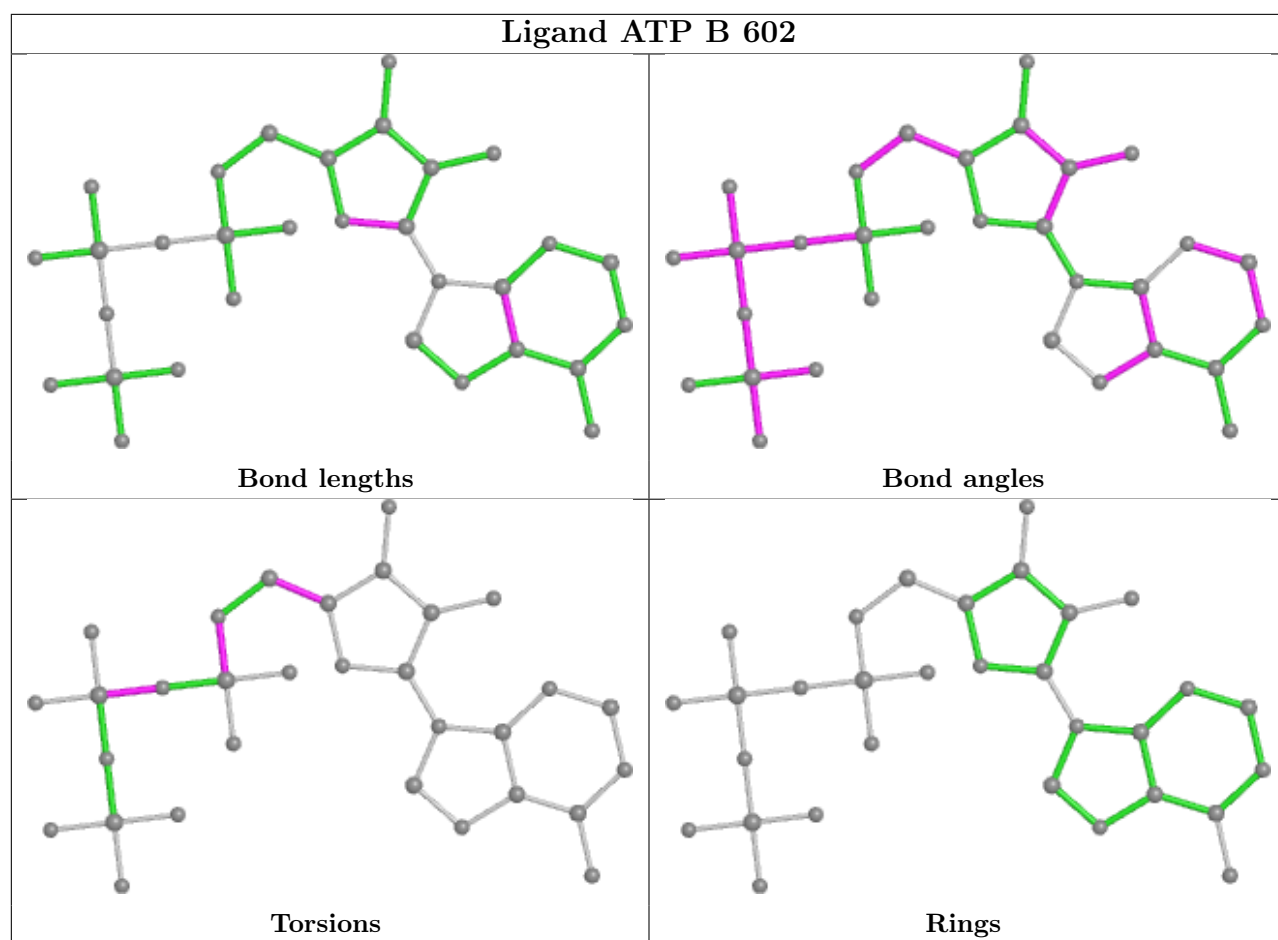
6 monomers are involved in 34 short contacts:

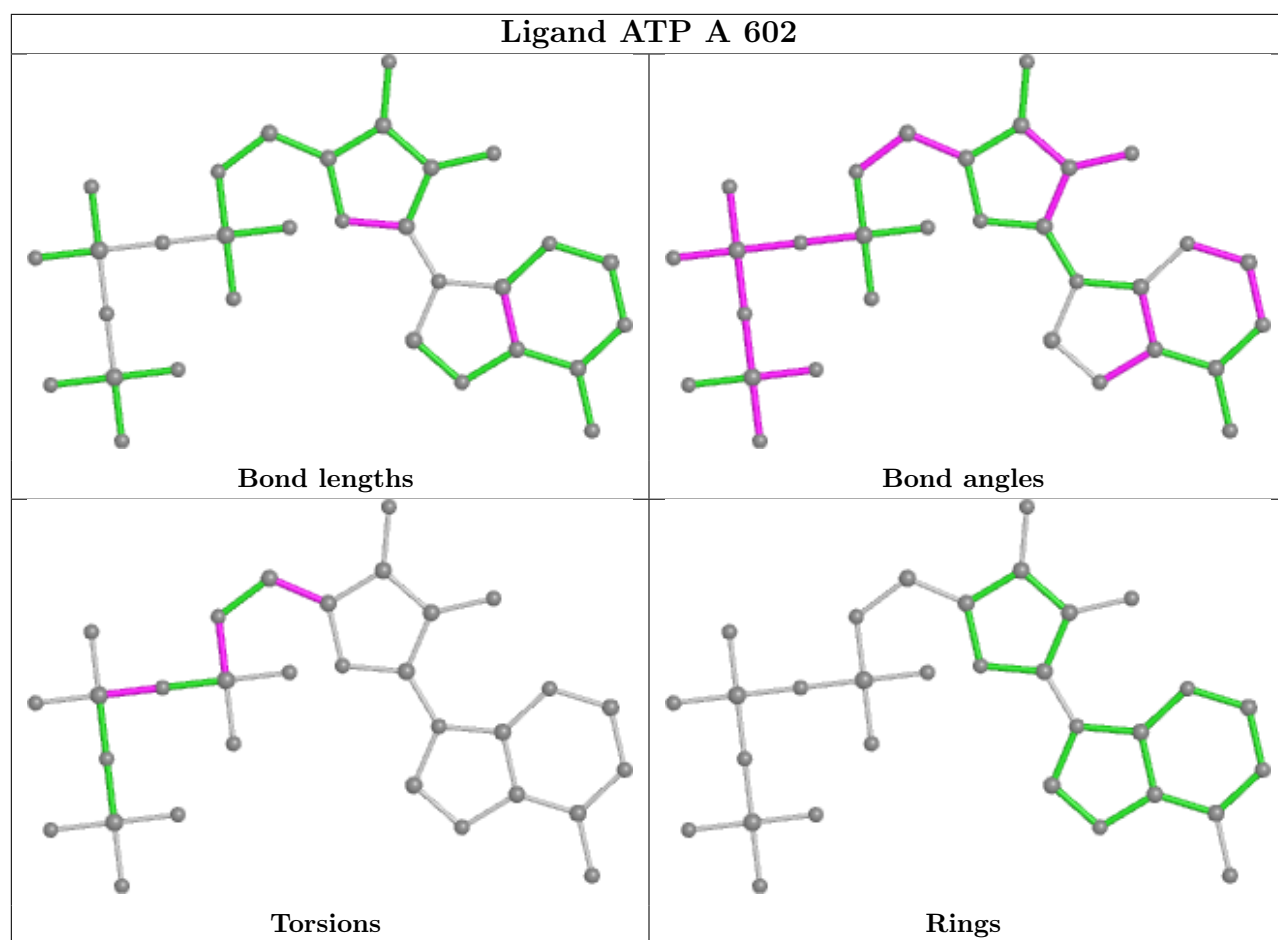
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	ATP	6	0
3	F	602	ATP	6	0
3	B	602	ATP	5	0
3	A	602	ATP	6	0
3	D	602	ATP	6	0
3	C	602	ATP	5	0

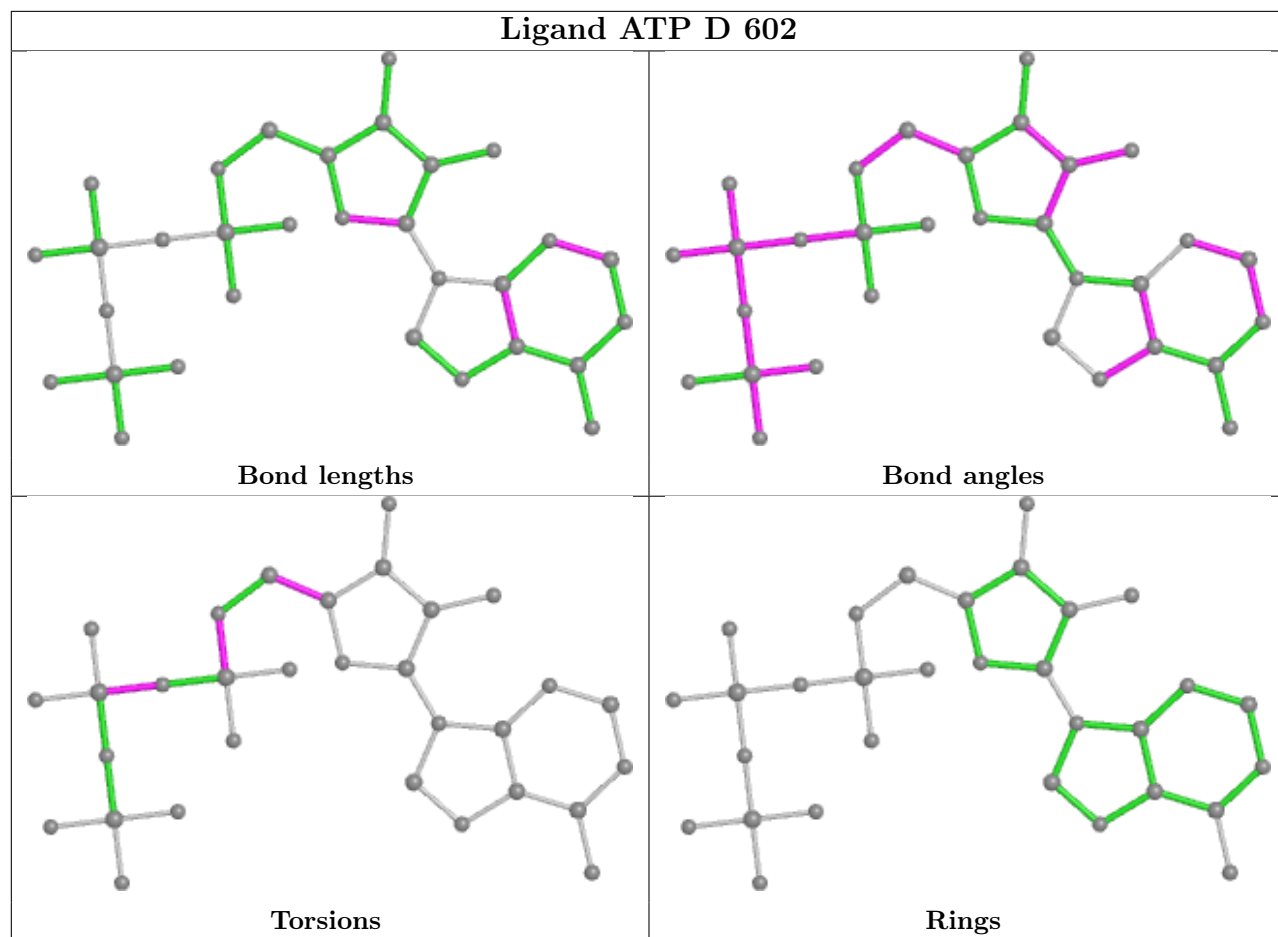
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

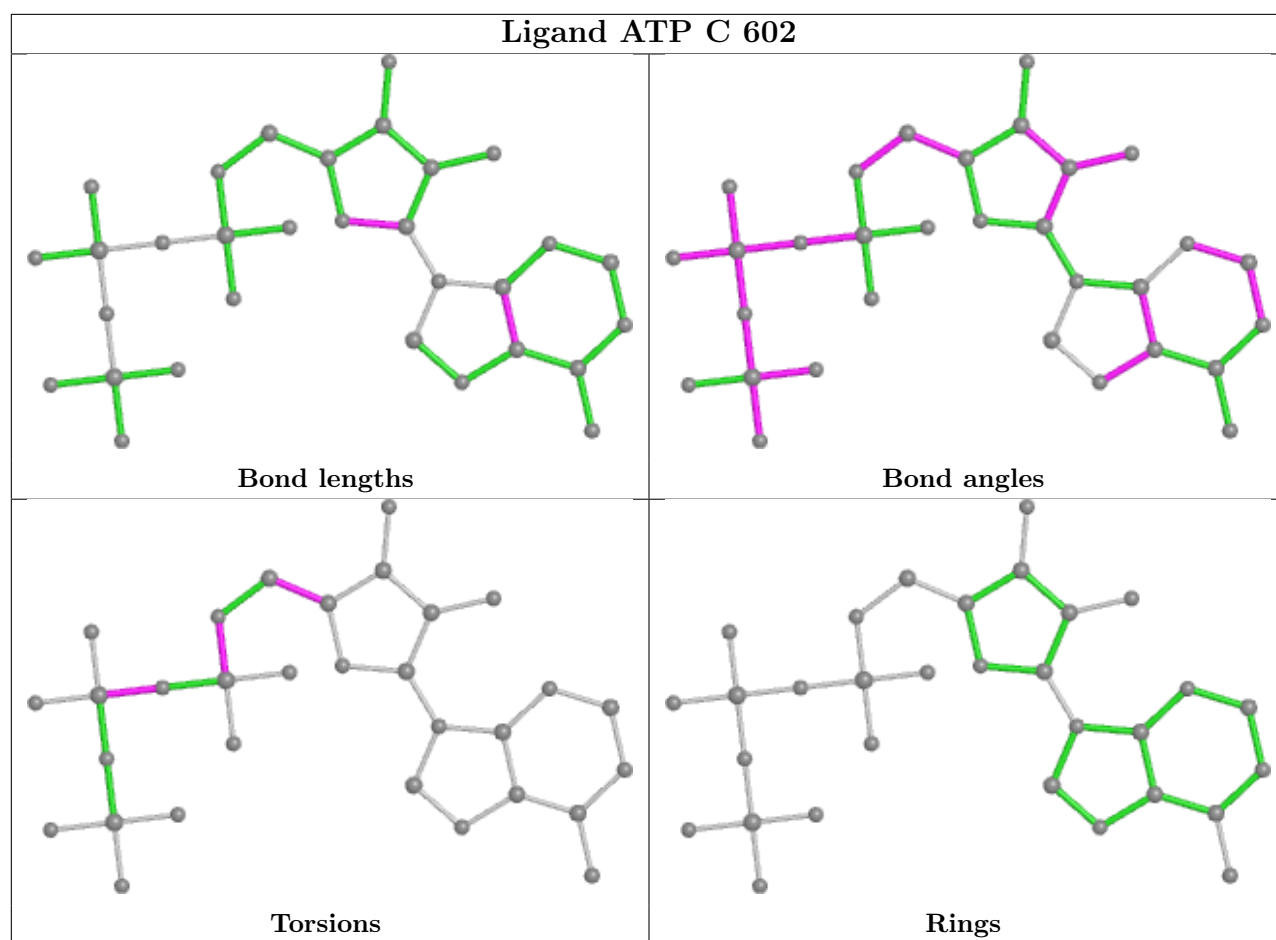












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

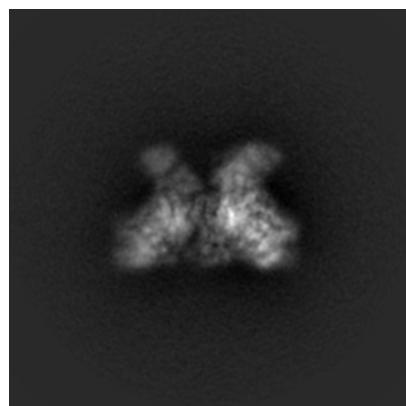
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36450. These allow visual inspection of the internal detail of the map and identification of artifacts.

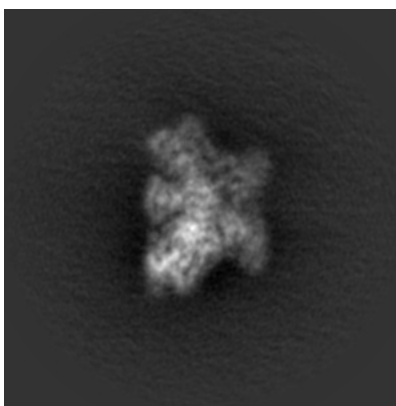
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

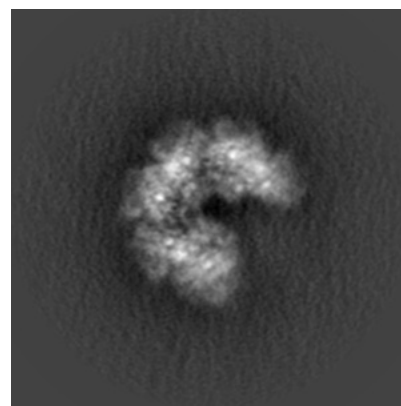
6.1.1 Primary map



X

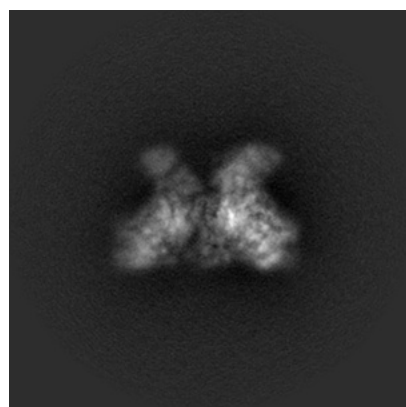


Y

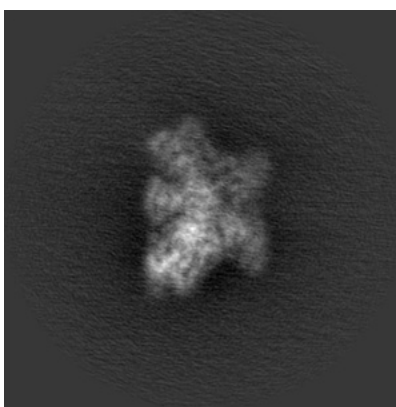


Z

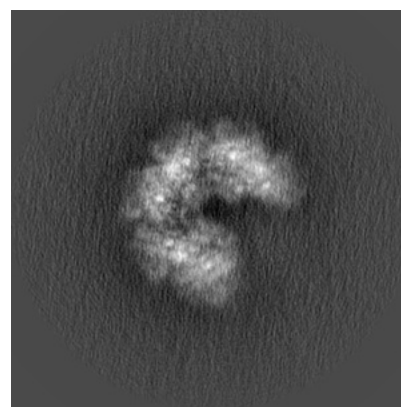
6.1.2 Raw map



X



Y

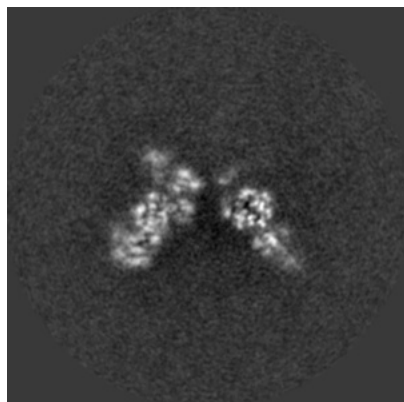


Z

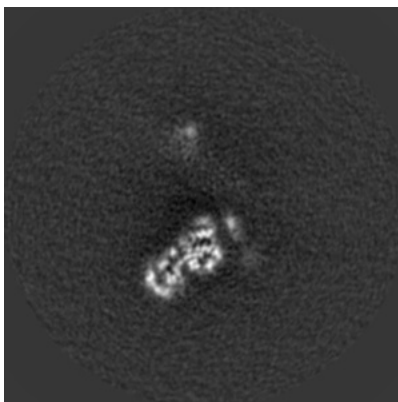
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

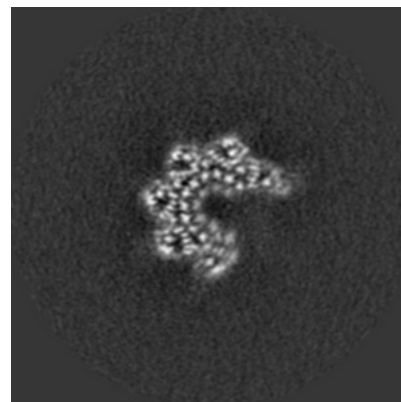
6.2.1 Primary map



X Index: 128

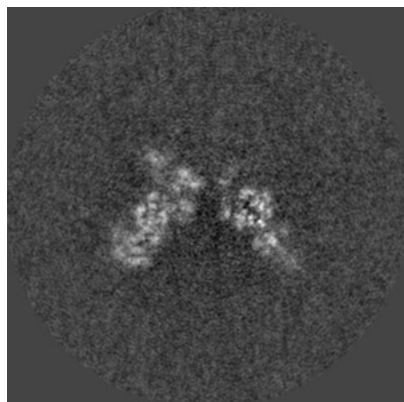


Y Index: 128

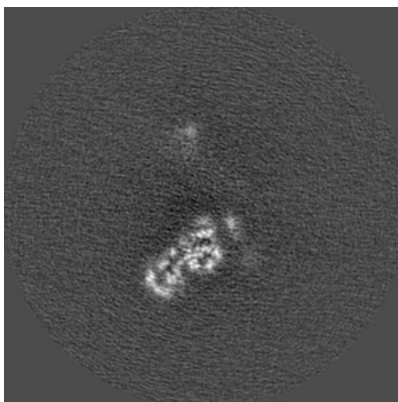


Z Index: 128

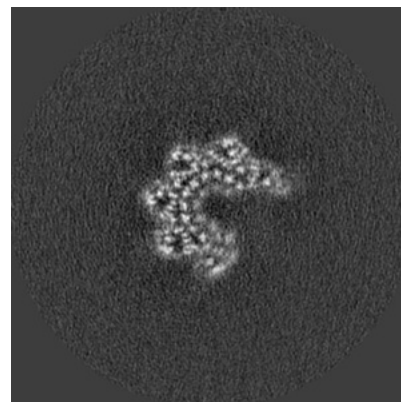
6.2.2 Raw map



X Index: 128



Y Index: 128

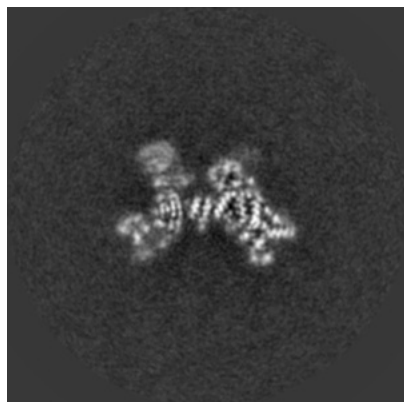


Z Index: 128

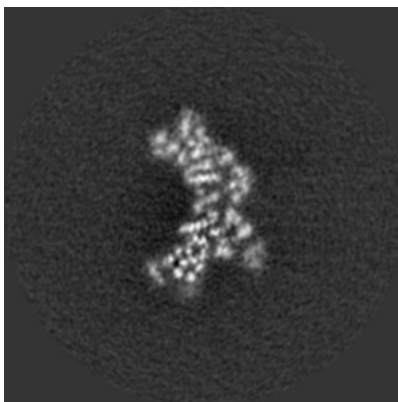
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

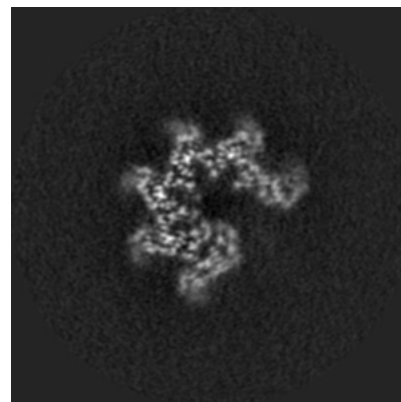
6.3.1 Primary map



X Index: 111

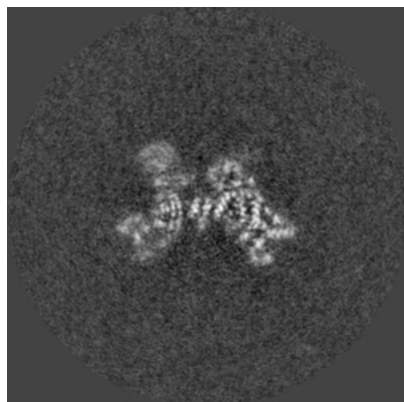


Y Index: 141

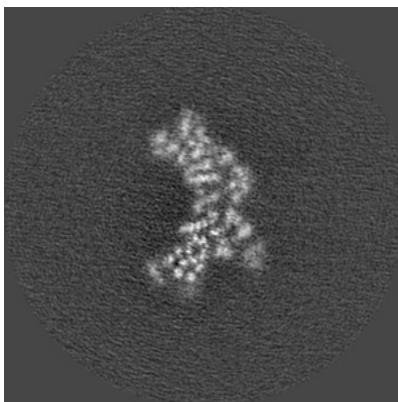


Z Index: 119

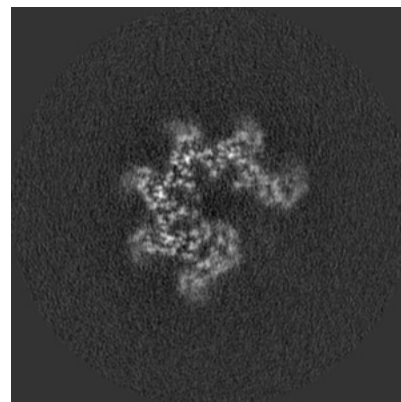
6.3.2 Raw map



X Index: 111



Y Index: 141



Z Index: 119

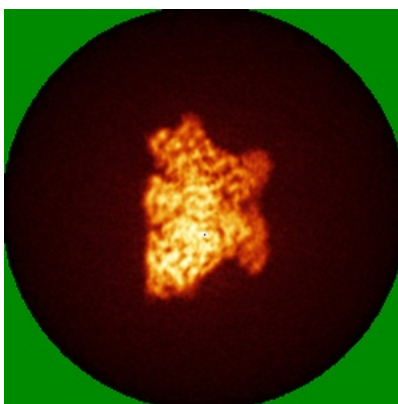
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

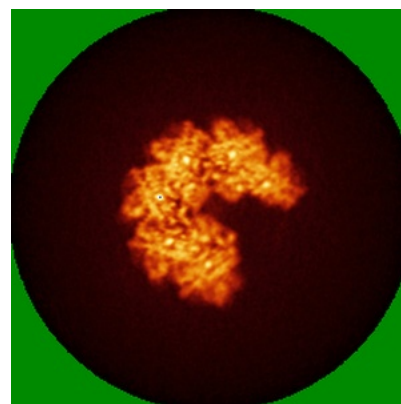
6.4.1 Primary map



X

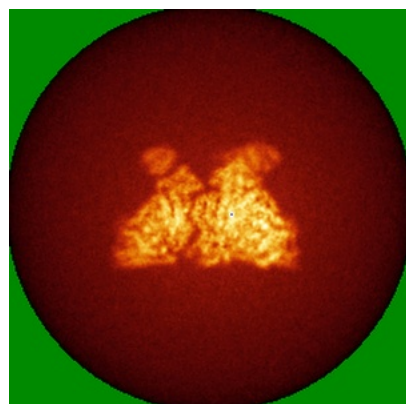


Y

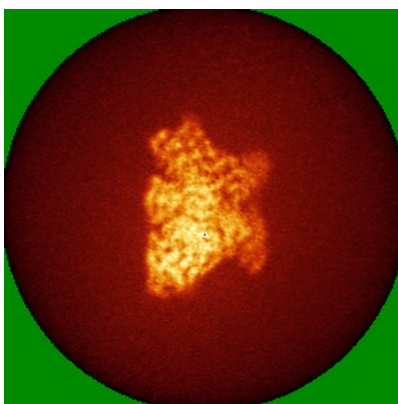


Z

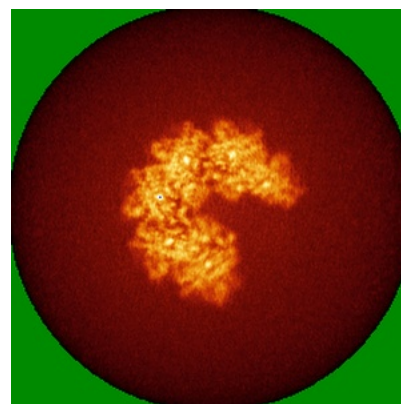
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

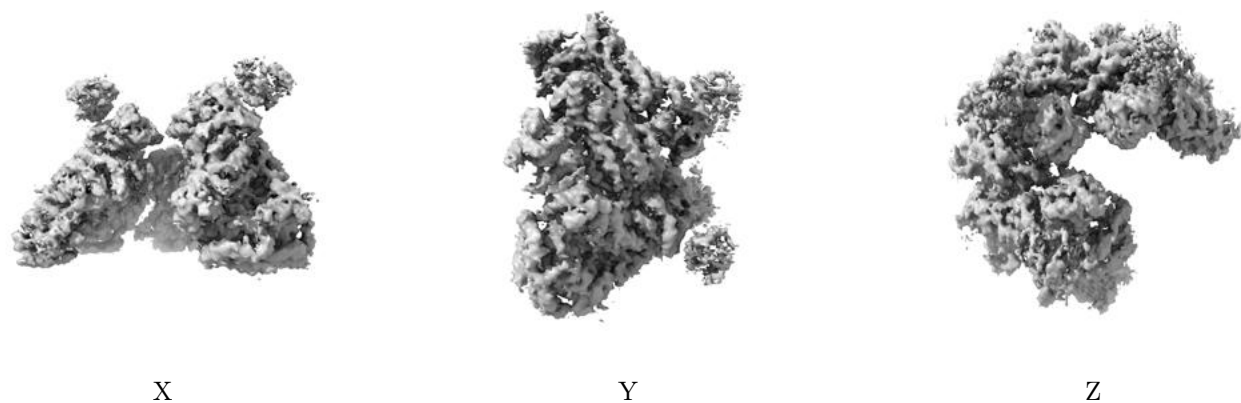
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

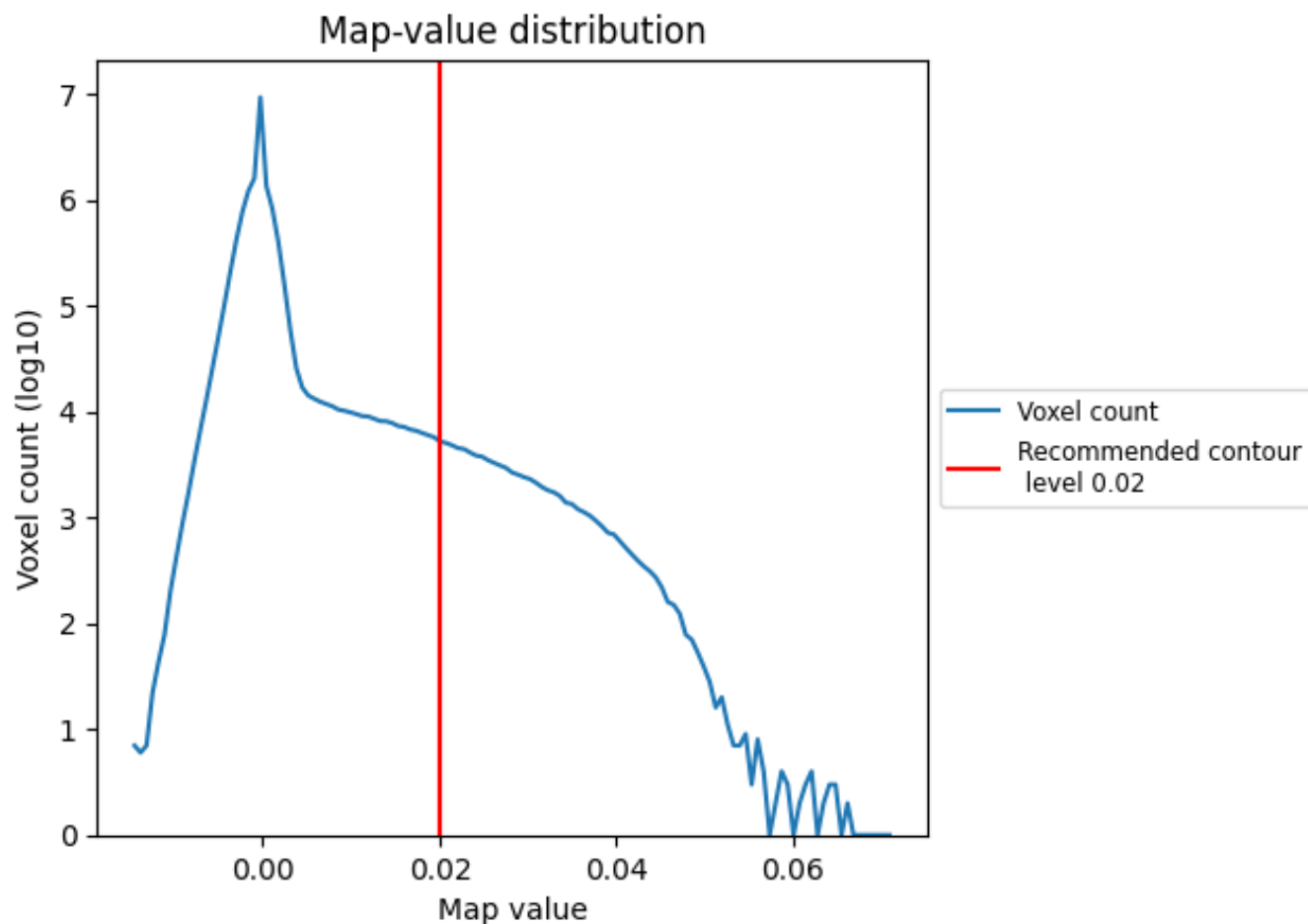
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

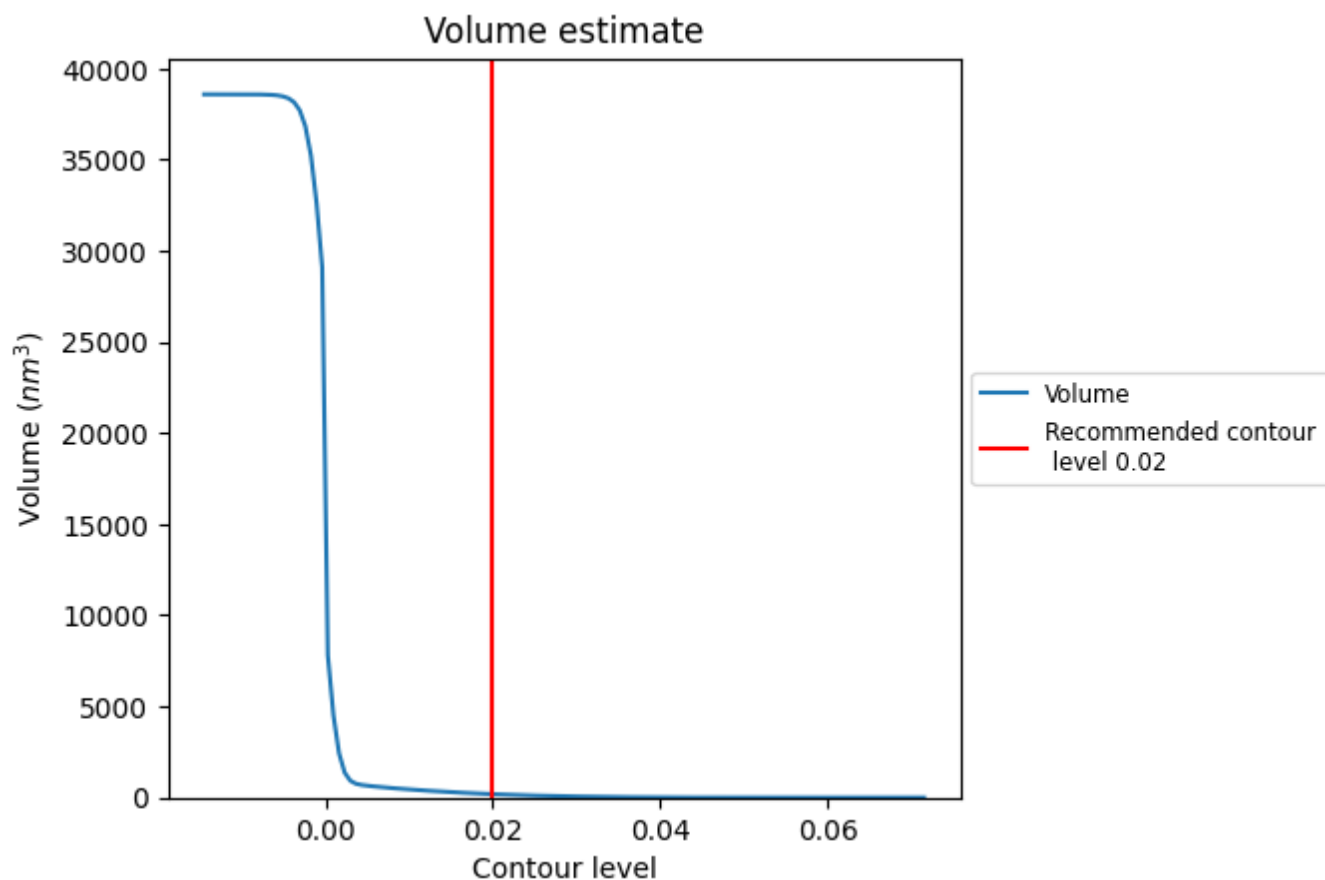
This section contains the results of statistical analysis of the map.

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.

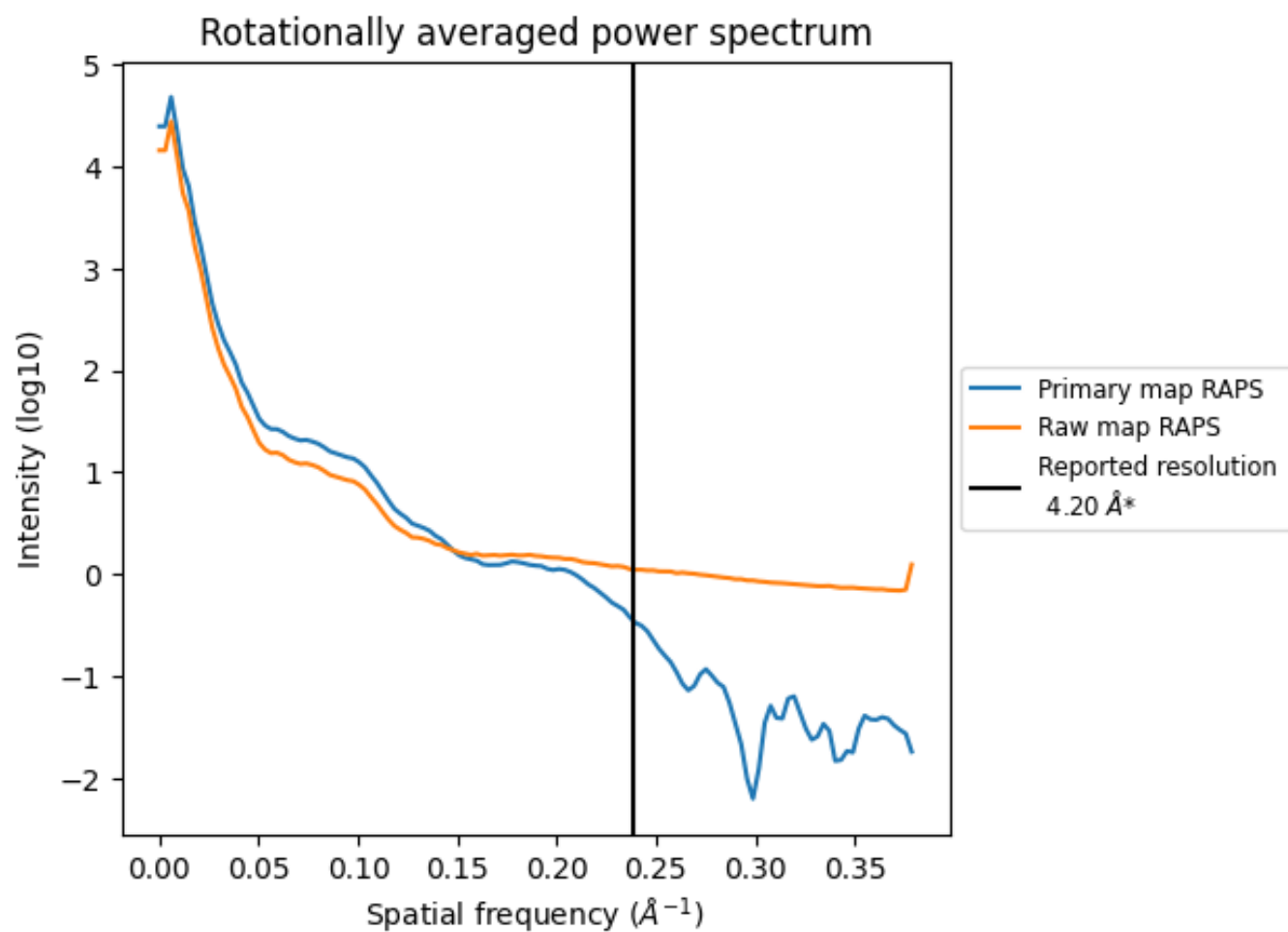
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 168 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 ⓘ

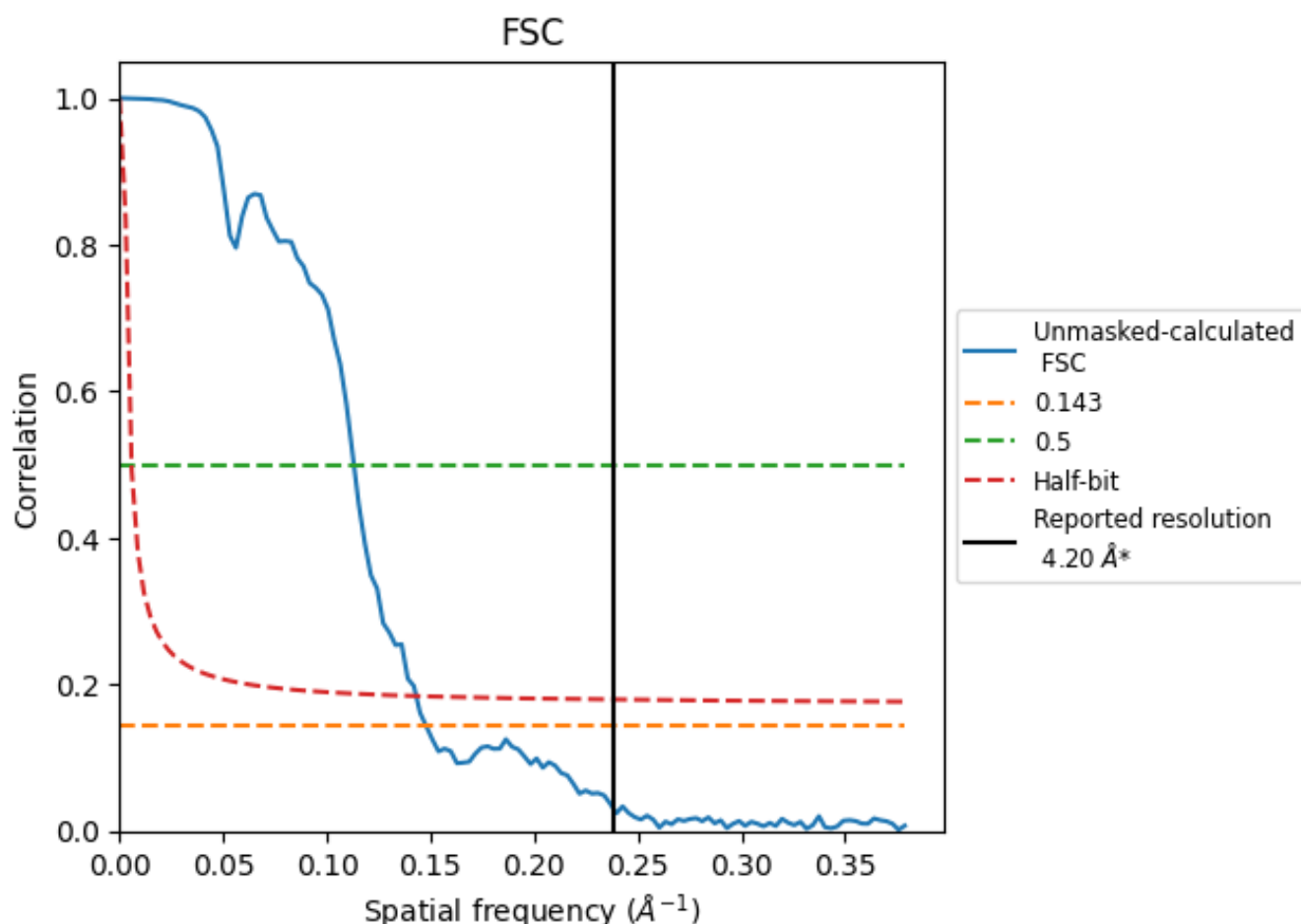


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

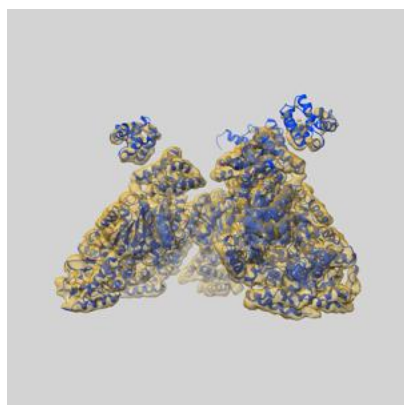
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.76	8.85	6.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.76 differs from the reported value 4.2 by more than 10 %

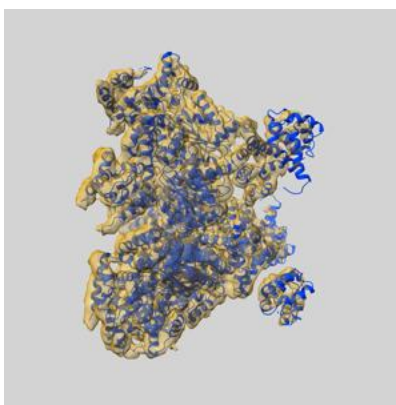
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36450 and PDB model 8JNS. Per-residue inclusion information can be found in section [3](#) on page [6](#).

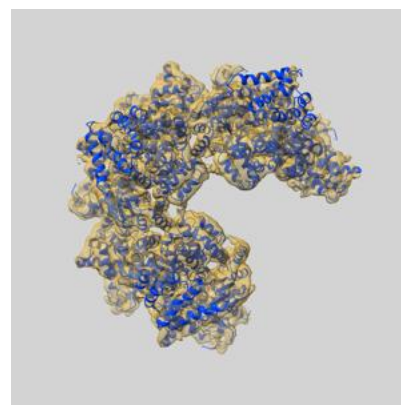
9.1 Map-model overlay [i](#)



X



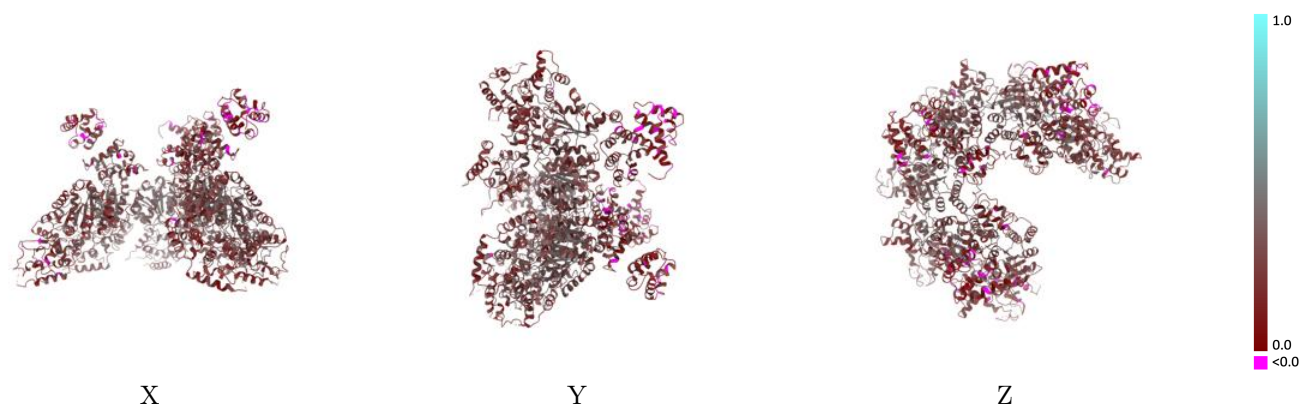
Y



Z

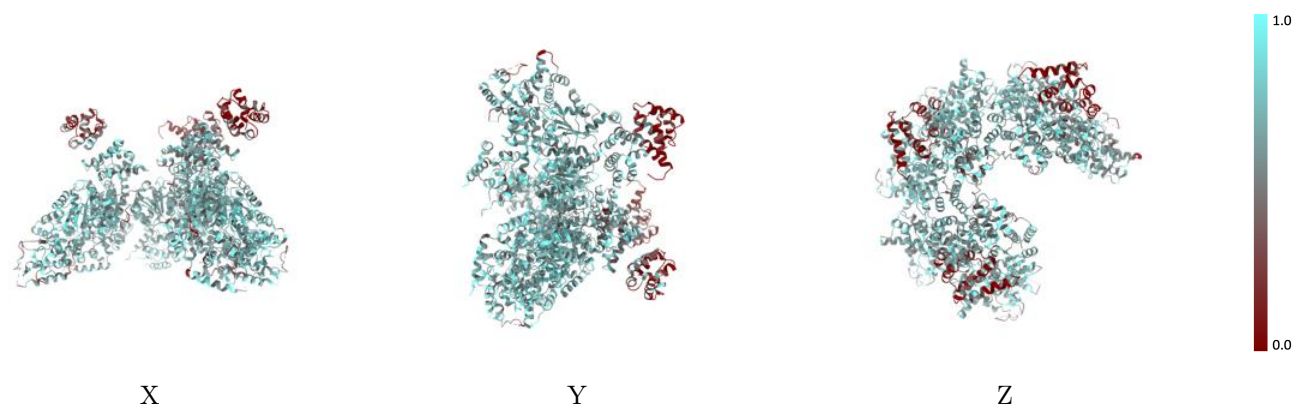
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



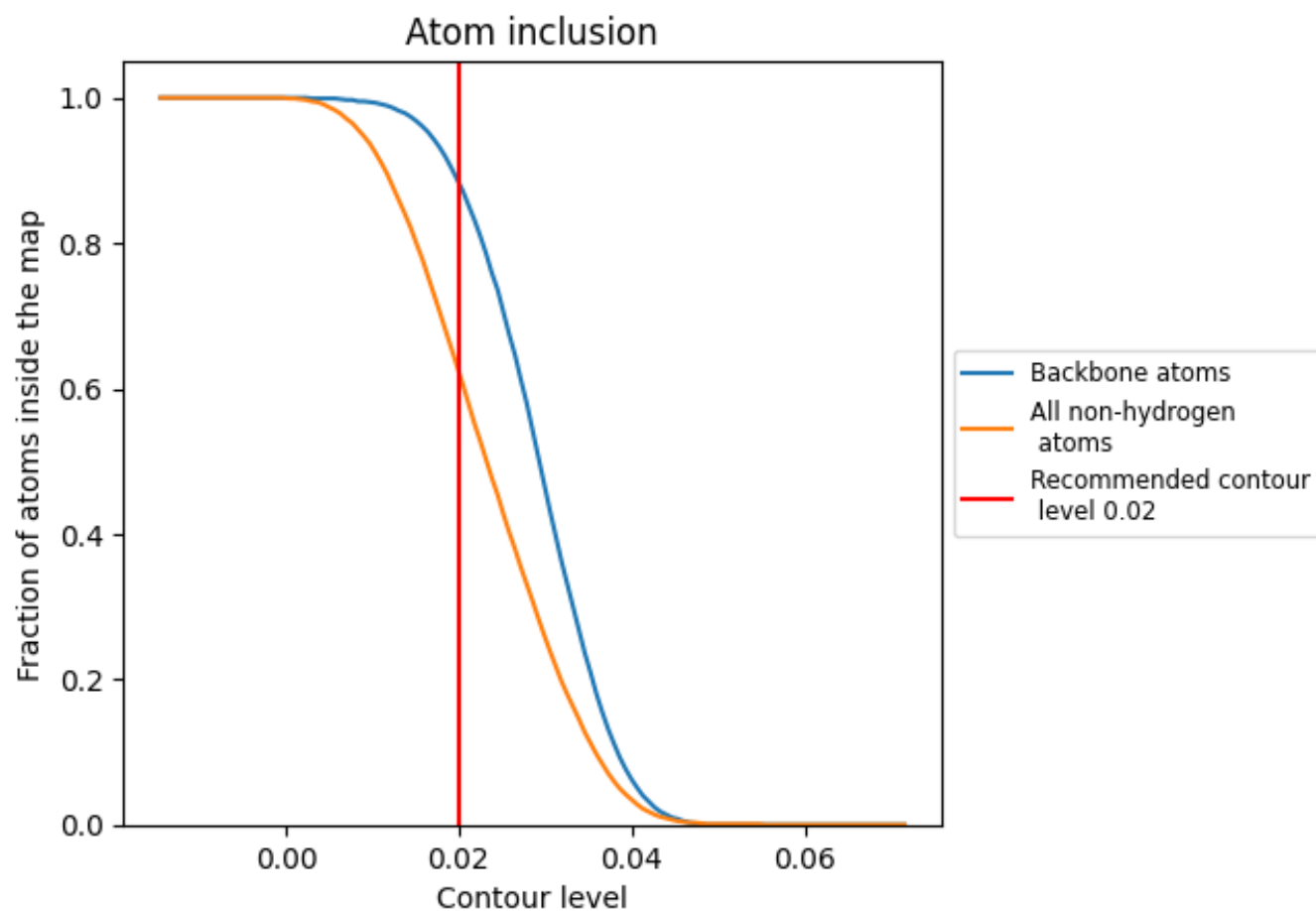
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 62% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6240	<div></div> 0.2630
A	<div></div> 0.6270	<div></div> 0.2510
B	<div></div> 0.6830	<div></div> 0.2850
C	<div></div> 0.6680	<div></div> 0.2850
D	<div></div> 0.6910	<div></div> 0.2990
E	<div></div> 0.6590	<div></div> 0.2430
F	<div></div> 0.7090	<div></div> 0.3130
G	<div></div> 0.2680	<div></div> 0.1310
H	<div></div> 0.1220	<div></div> 0.1130
I	<div></div> 0.2280	<div></div> 0.1500

1.0

0.0

<0.0