



Full wwPDB EM Validation Report ⓘ

Aug 25, 2024 – 12:22 AM JST

PDB ID : 8XUV
EMDB ID : EMD-38685
Title : Cryo-EM structure of tomato NRC2 filament
Authors : Sun, Y.; Ma, S.C.; Chai, J.J.
Deposited on : 2024-01-14
Resolution : 3.60 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:

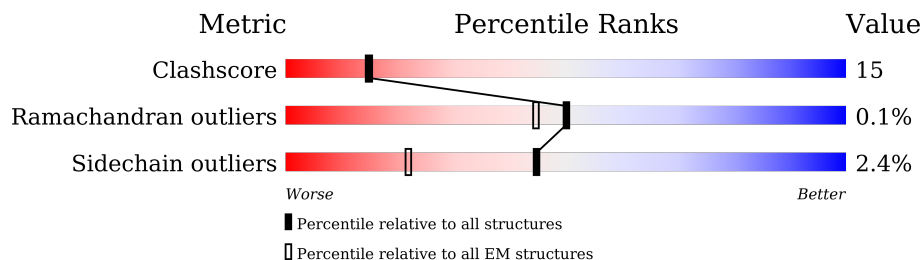
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	885	
1	B	885	
1	C	885	
1	D	885	
1	E	885	
1	F	885	
1	G	885	
1	H	885	
1	I	885	

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Mol	Chain	Length	Quality of chain	
1	J	885	 68%	31%
1	K	885	 69%	30%
1	L	885	 71%	28%

2 Entry composition i

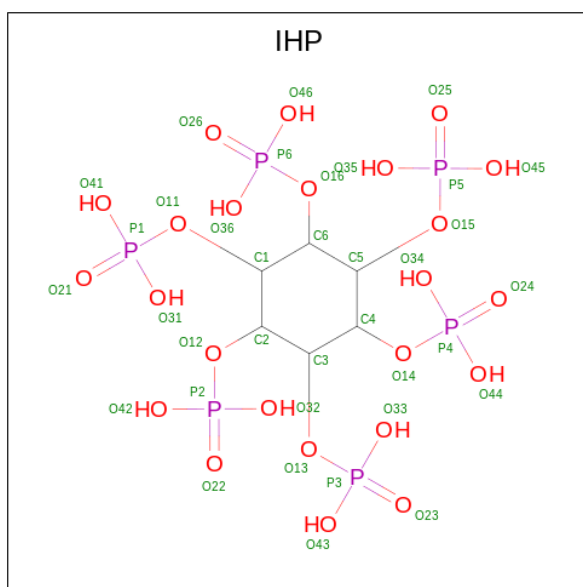
There are 3 unique types of molecules in this entry. The entry contains 86208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	885	7121	4544	1237	1308	32	0	0
1	B	885	7121	4544	1237	1308	32	0	0
1	C	885	7121	4544	1237	1308	32	0	0
1	D	885	7121	4544	1237	1308	32	0	0
1	E	885	7121	4544	1237	1308	32	0	0
1	F	885	7121	4544	1237	1308	32	0	0
1	G	885	7121	4544	1237	1308	32	0	0
1	H	885	7121	4544	1237	1308	32	0	0
1	I	885	7121	4544	1237	1308	32	0	0
1	J	885	7121	4544	1237	1308	32	0	0
1	K	885	7121	4544	1237	1308	32	0	0
1	L	885	7121	4544	1237	1308	32	0	0

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
2	A	1	36	6	24	6	0
2	B	1	36	6	24	6	0
2	C	1	36	6	24	6	0
2	D	1	36	6	24	6	0
2	E	1	36	6	24	6	0
2	F	1	36	6	24	6	0
2	G	1	36	6	24	6	0
2	H	1	36	6	24	6	0
2	I	1	36	6	24	6	0
2	J	1	36	6	24	6	0
2	K	1	36	6	24	6	0
2	L	1	36	6	24	6	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

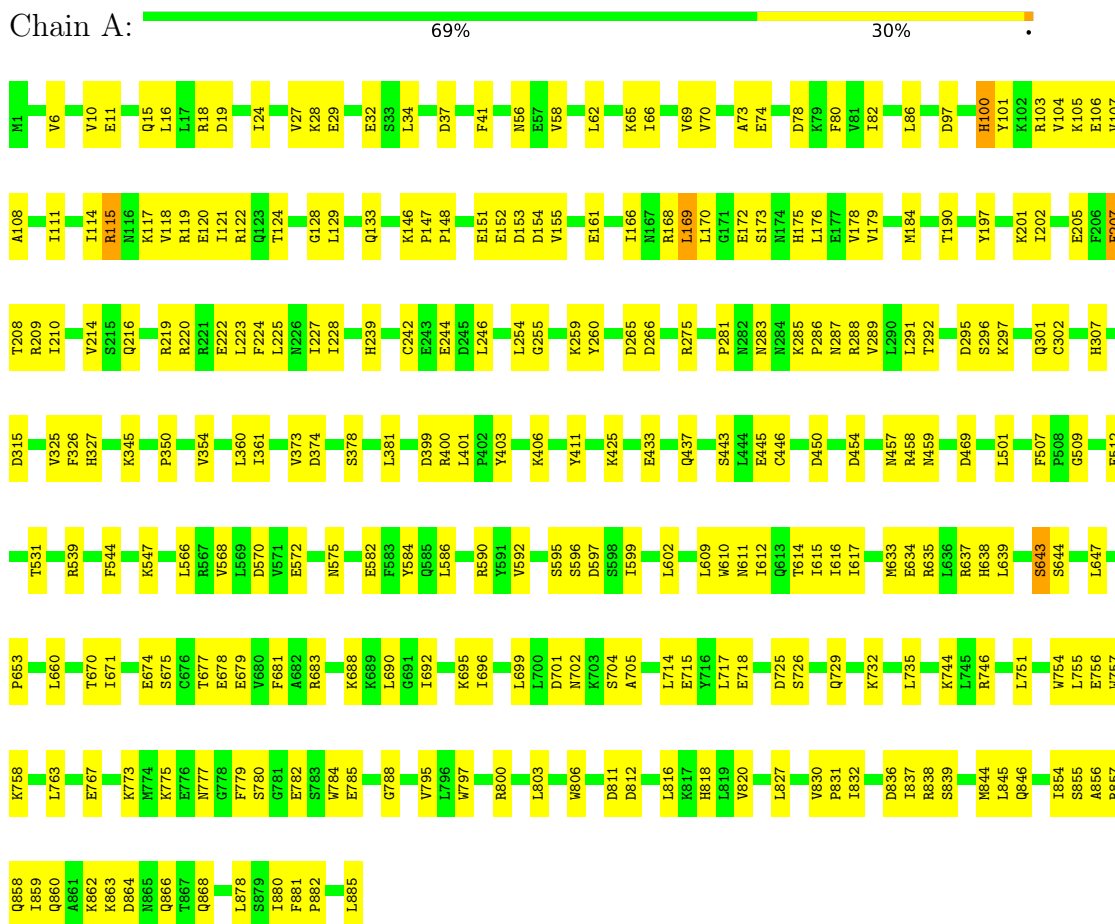


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

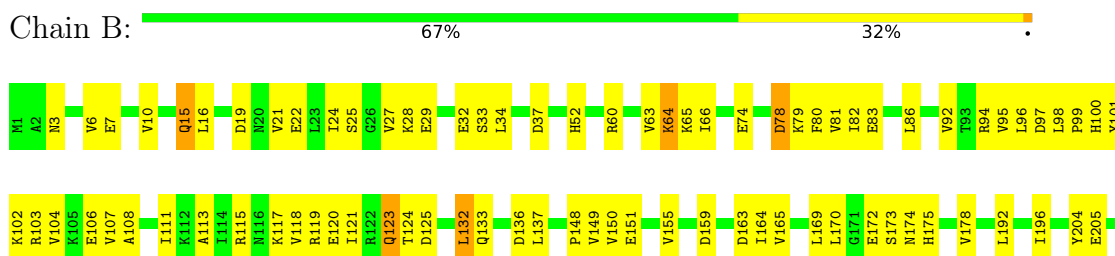
3 Residue-property plots [i](#)

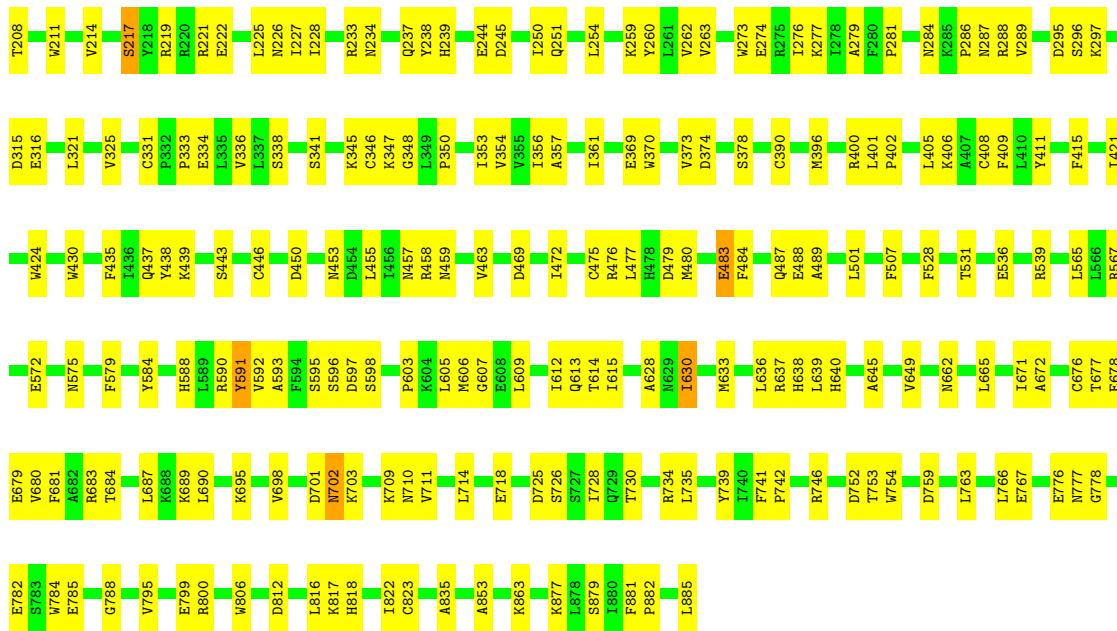
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NRC2

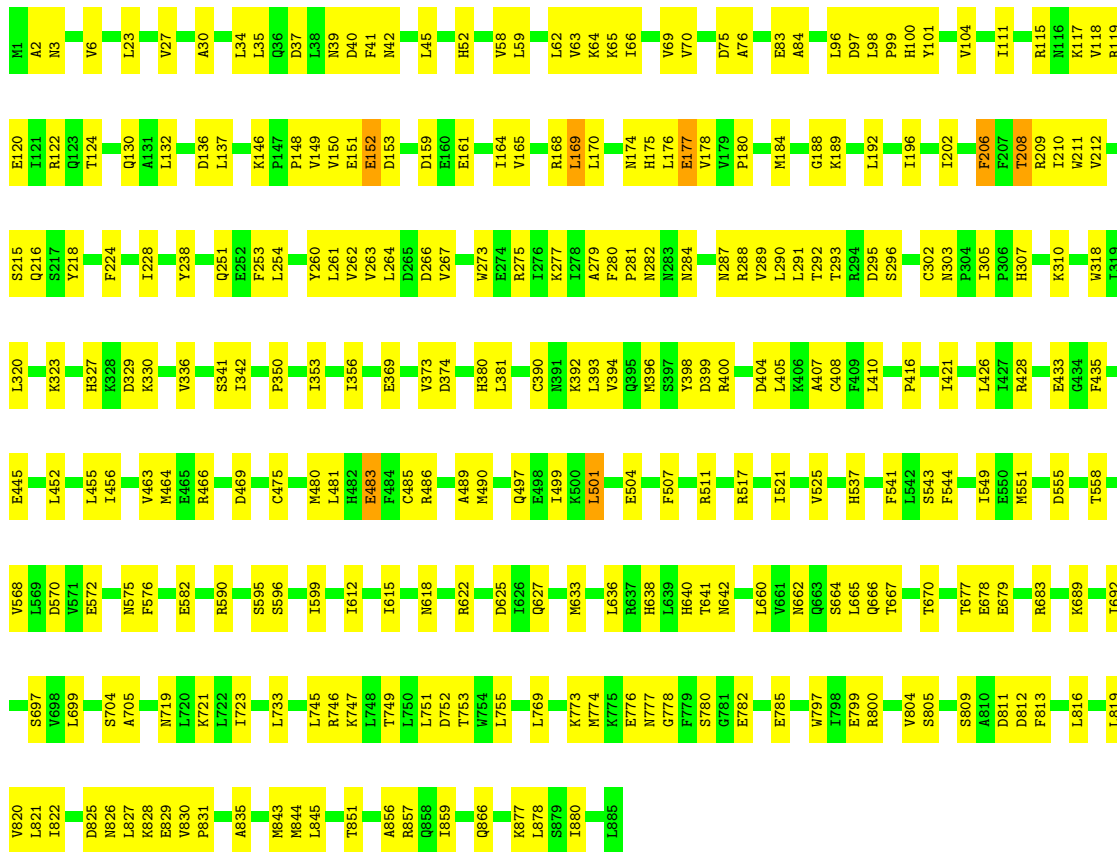


- Molecule 1: NRC2



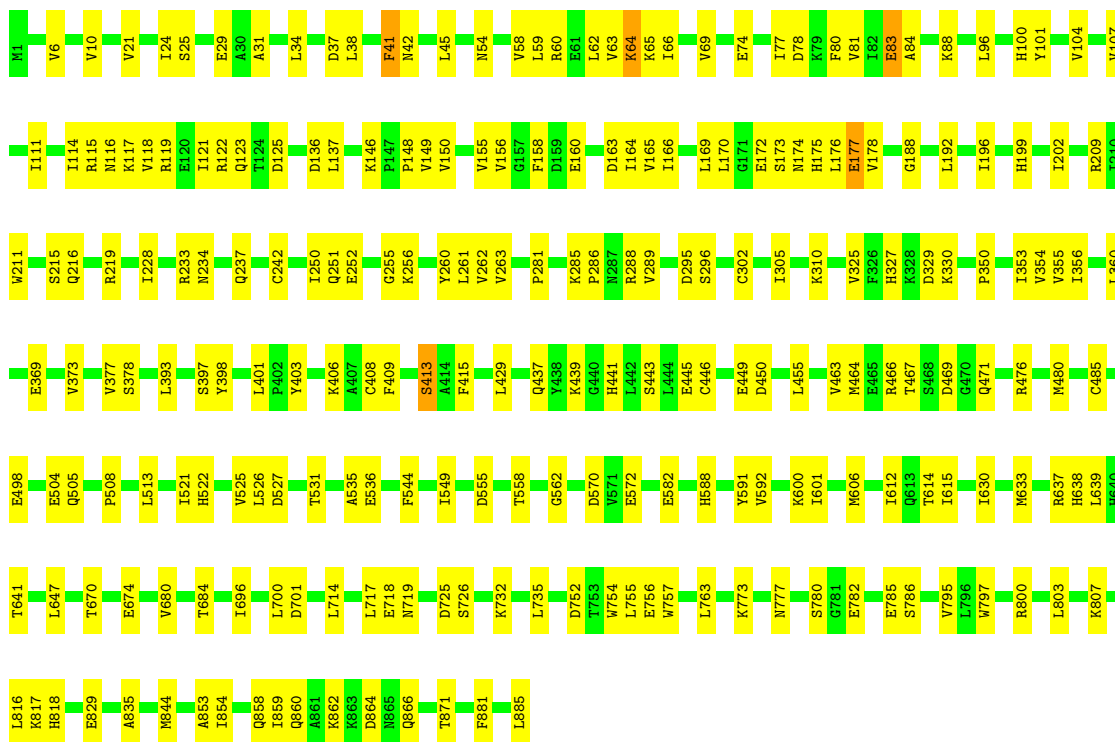


• Molecule 1: NRC2



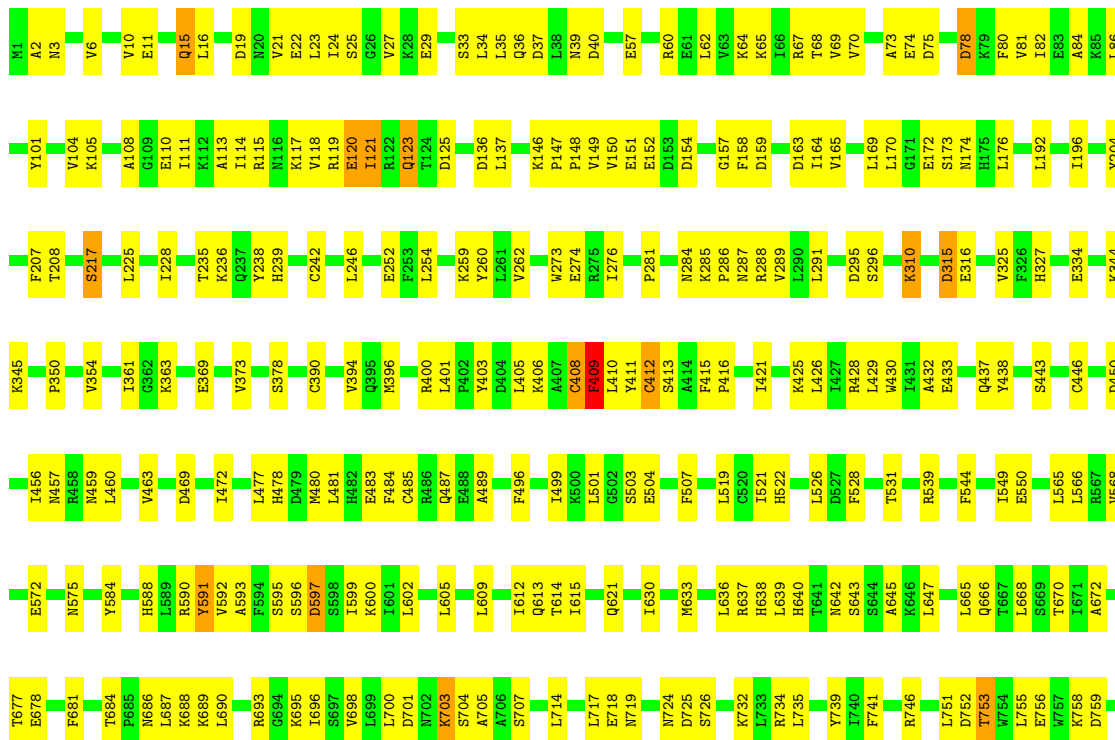
• Molecule 1: NRC2

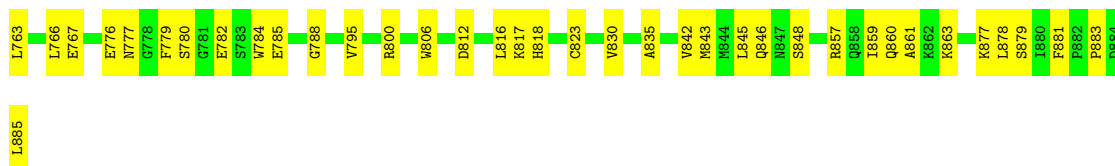
Chain D: 74% 26%



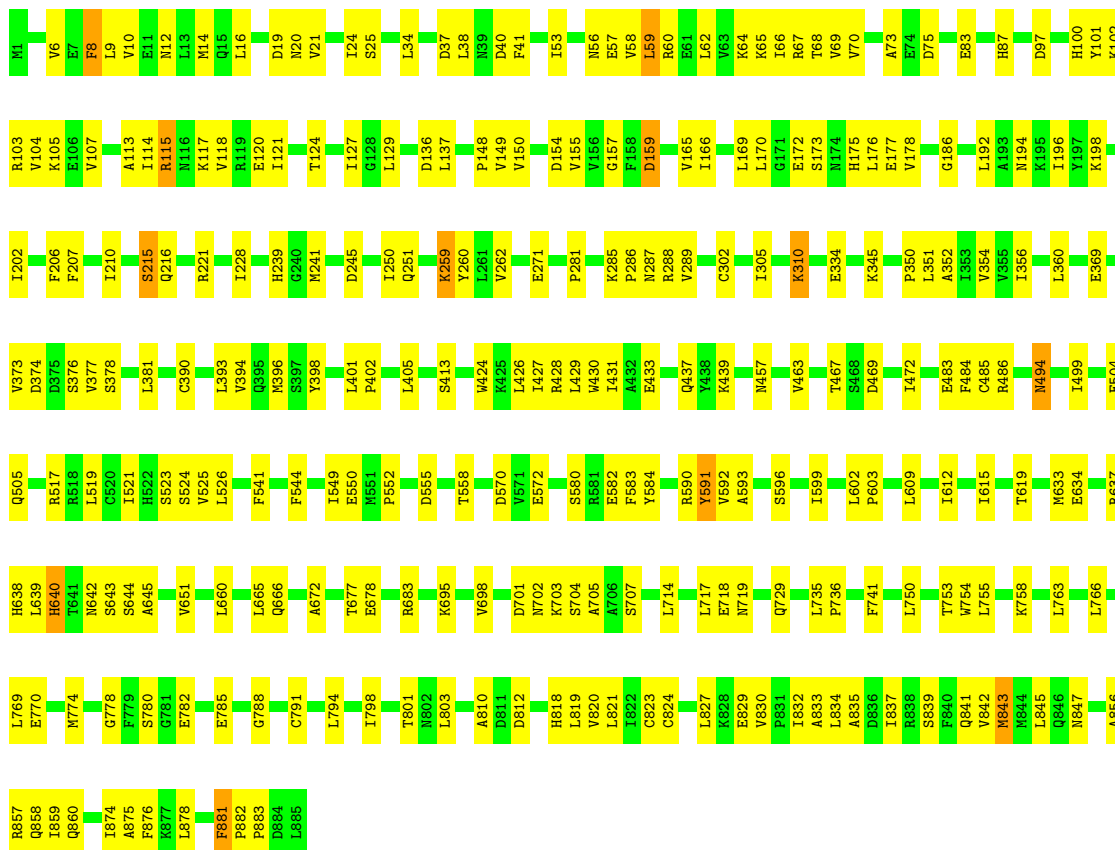
• Molecule 1: NRC2

Chain E: 66% 32%

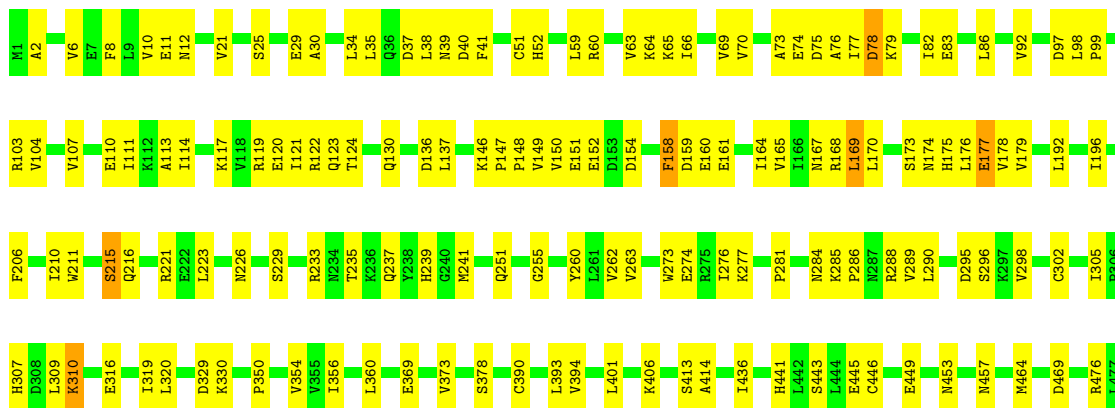


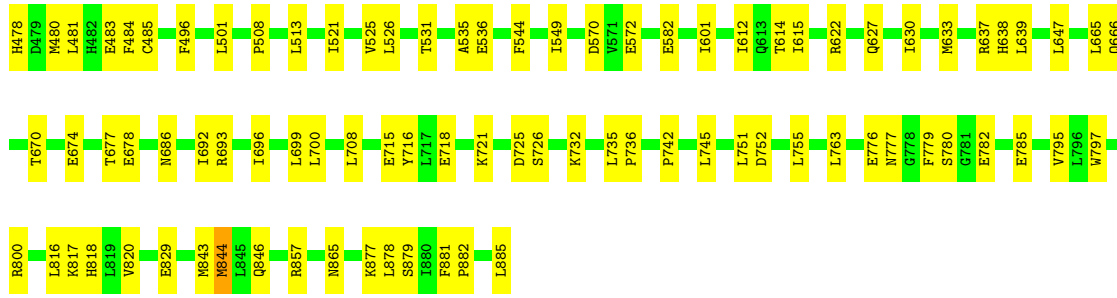


• Molecule 1: NRC2

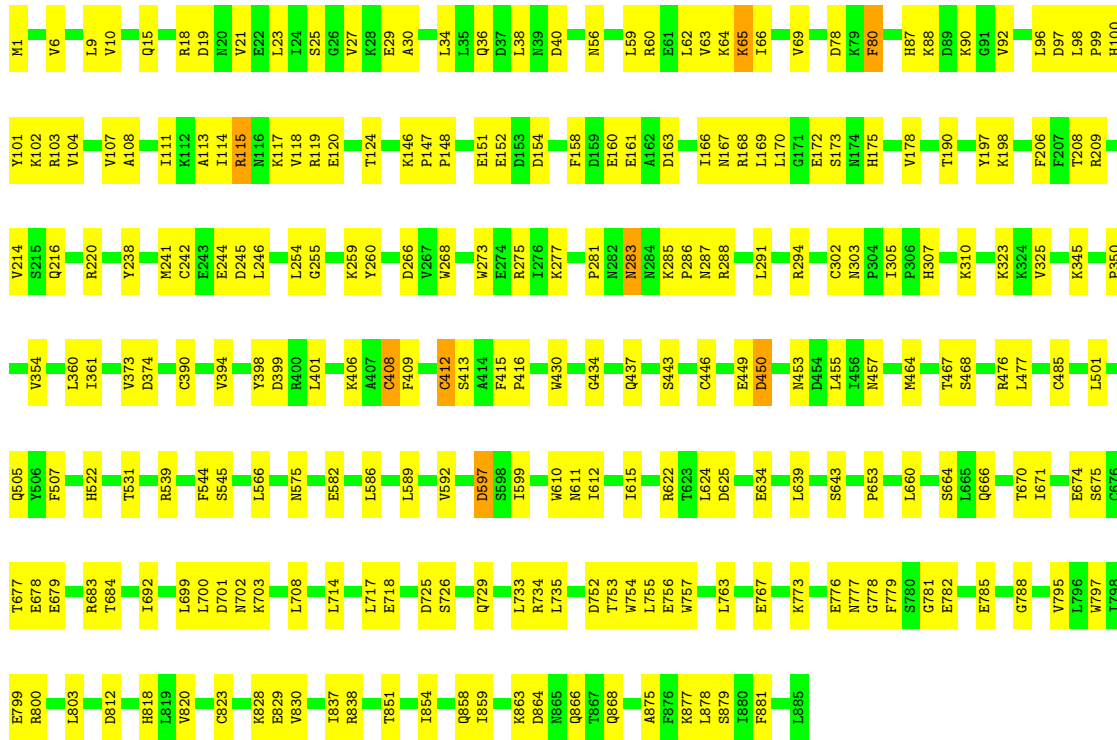


• Molecule 1: NRC2

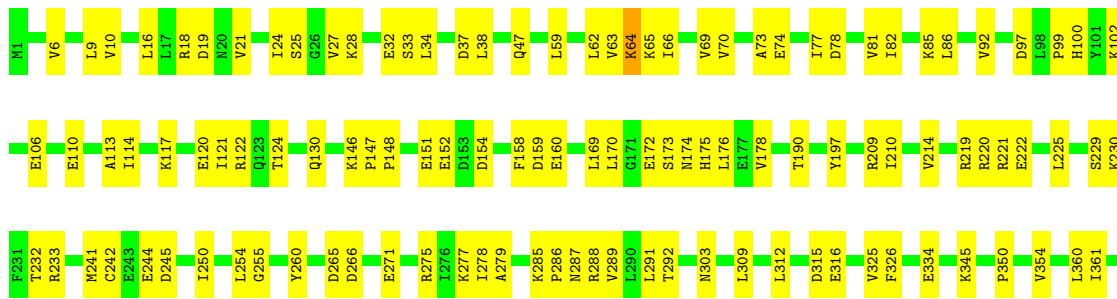


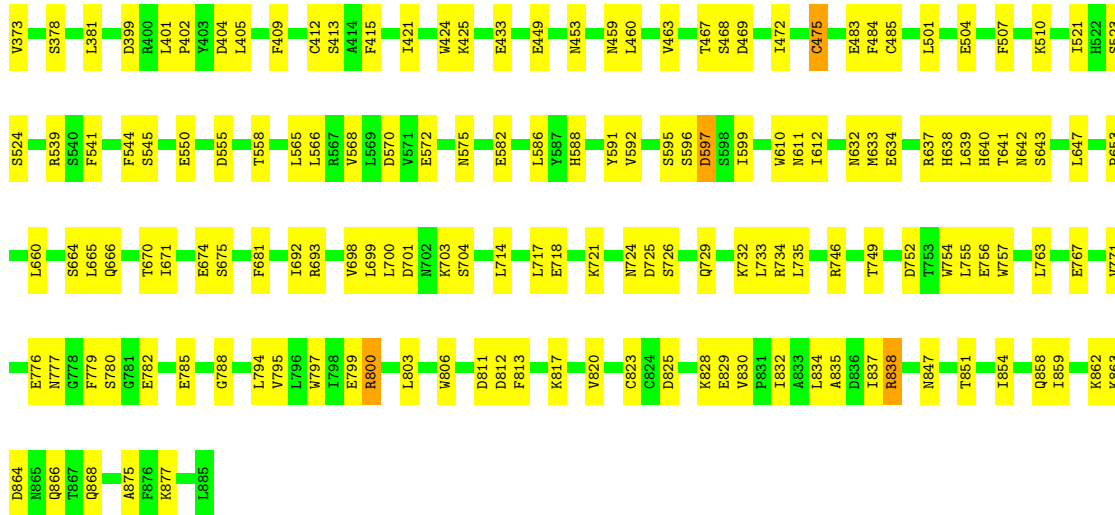


• Molecule 1: NRC2

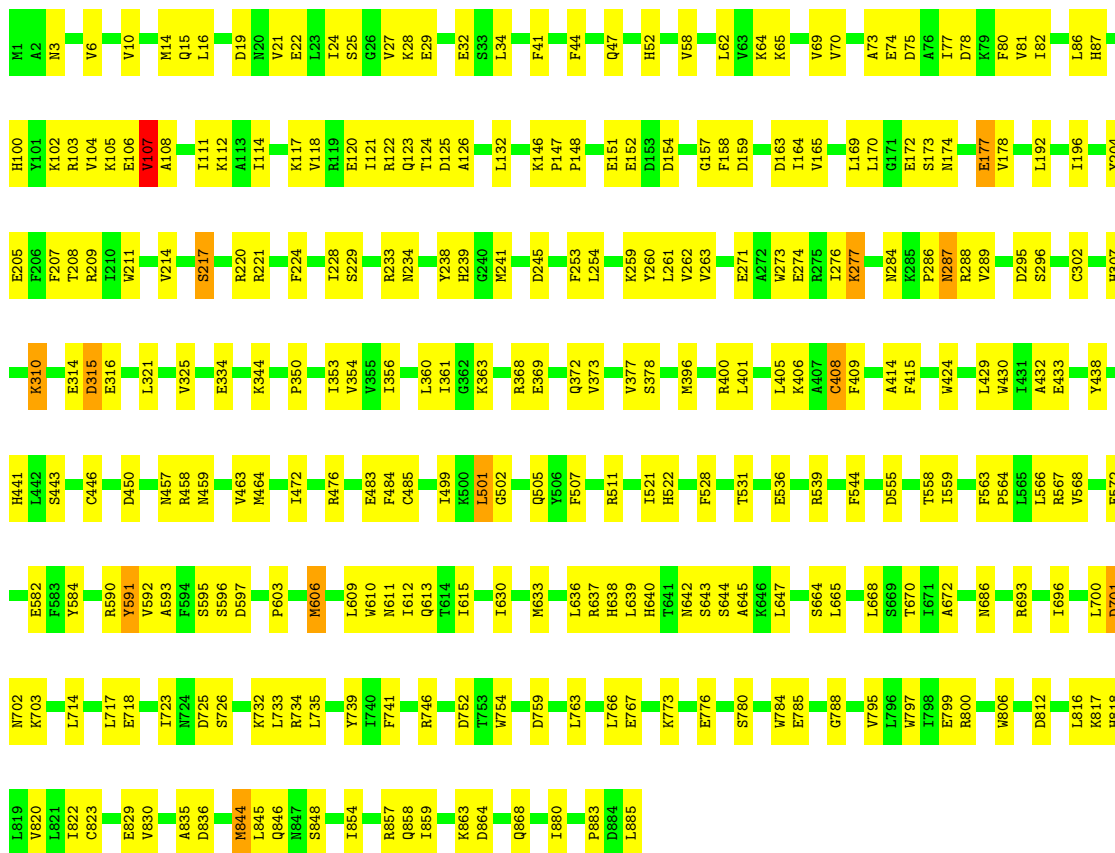


• Molecule 1: NRC2



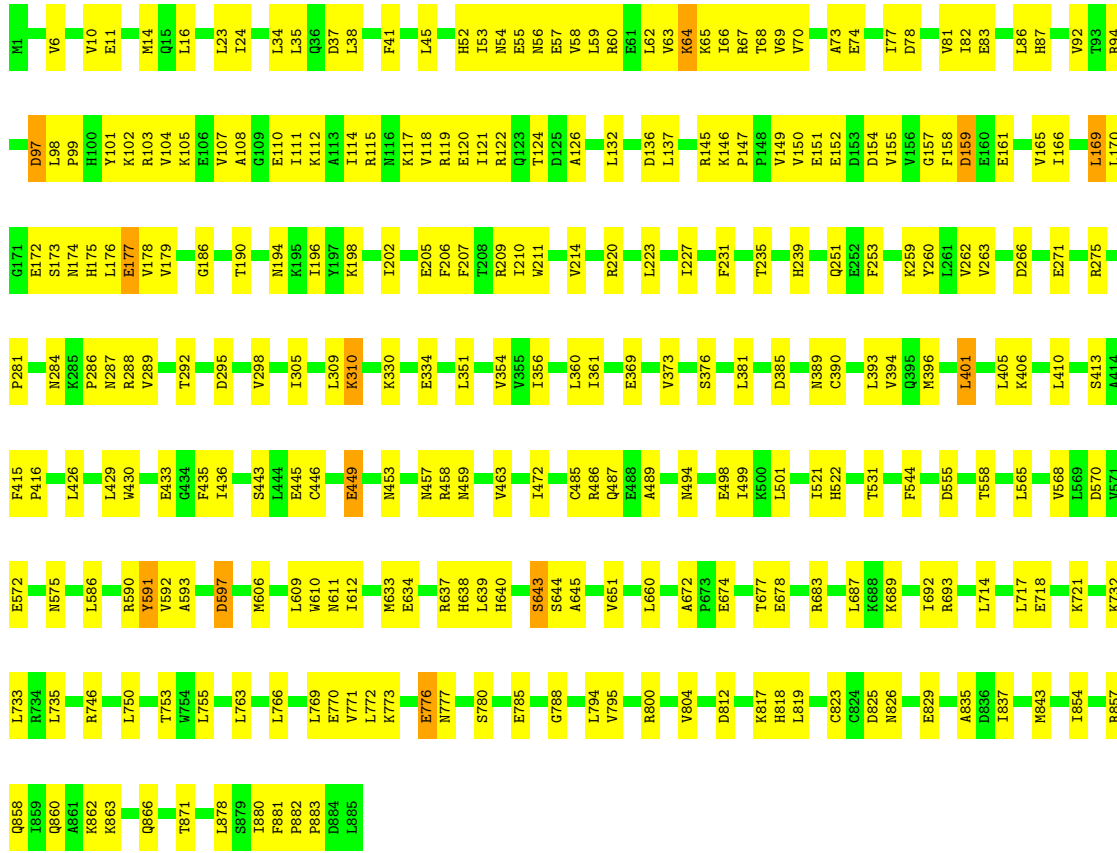


• Molecule 1: NRC2

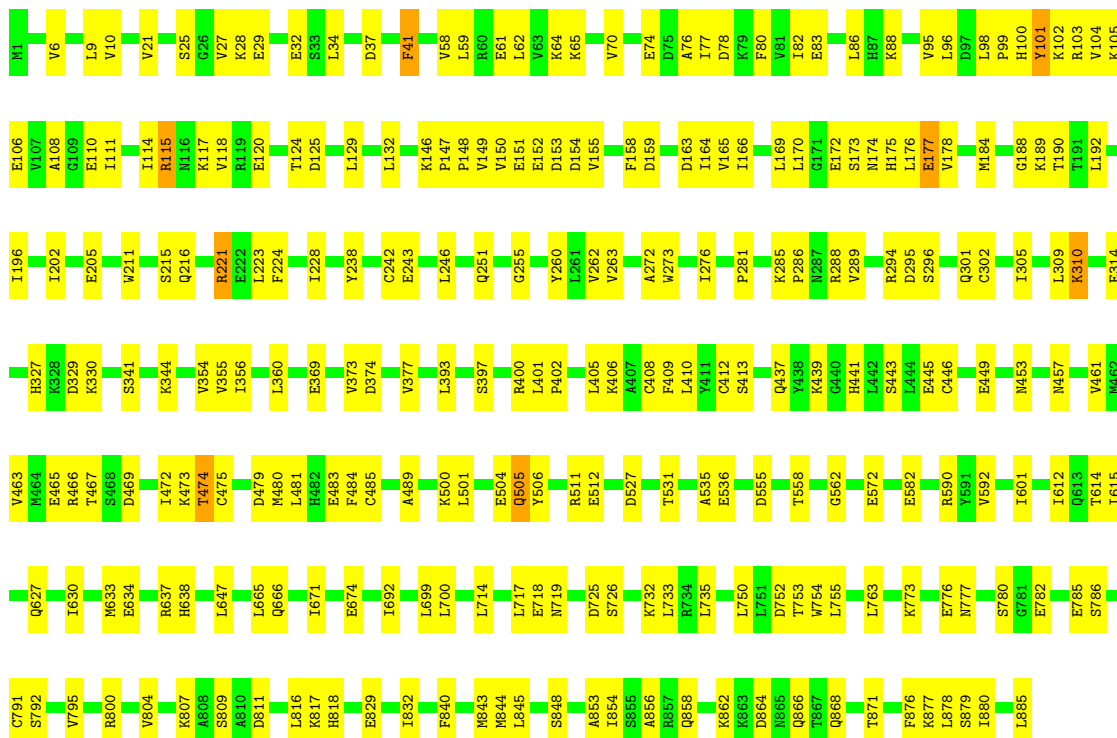


• Molecule 1: NRC2





• Molecule 1: NRC2



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-55.85°, rise=64.04 Å, axial sym=C3	Depositor
Number of segments used	280426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/7260	0.51	0/9803
1	B	0.34	0/7260	0.54	0/9803
1	C	0.30	0/7260	0.54	0/9803
1	D	0.30	0/7260	0.51	0/9803
1	E	0.33	0/7260	0.52	0/9803
1	F	0.31	0/7260	0.52	0/9803
1	G	0.31	0/7260	0.51	0/9803
1	H	0.32	0/7260	0.53	0/9803
1	I	0.32	0/7260	0.51	0/9803
1	J	0.32	0/7260	0.52	0/9803
1	K	0.33	0/7260	0.53	0/9803
1	L	0.30	0/7260	0.51	0/9803
All	All	0.32	0/87120	0.52	0/117636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7121	0	7283	225	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7121	0	7283	232	0
1	C	7121	0	7283	210	0
1	D	7121	0	7283	190	0
1	E	7121	0	7283	236	0
1	F	7121	0	7283	233	0
1	G	7121	0	7283	176	0
1	H	7121	0	7283	193	0
1	I	7121	0	7283	227	0
1	J	7121	0	7283	213	0
1	K	7121	0	7283	249	0
1	L	7121	0	7283	214	0
2	A	36	0	6	0	0
2	B	36	0	6	0	0
2	C	36	0	6	0	0
2	D	36	0	6	1	0
2	E	36	0	6	0	0
2	F	36	0	6	0	0
2	G	36	0	6	0	0
2	H	36	0	6	2	0
2	I	36	0	6	2	0
2	J	36	0	6	0	0
2	K	36	0	6	1	0
2	L	36	0	6	1	0
3	A	27	0	12	5	0
3	B	27	0	12	4	0
3	C	27	0	12	3	0
3	D	27	0	12	6	0
3	E	27	0	12	1	0
3	F	27	0	12	4	0
3	G	27	0	12	1	0
3	H	27	0	12	3	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	4	0
3	L	27	0	12	7	0
All	All	86208	0	87612	2593	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 15.

All (2593) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LEU:O	1:H:38:LEU:HD12	1.40	1.19
1:B:169:LEU:HD12	1:B:170:LEU:HG	1.26	1.07
1:B:254:LEU:HD11	1:B:260:TYR:CG	1.90	1.07
1:A:634:GLU:OE1	1:A:635:ARG:NH2	1.88	1.06
1:B:169:LEU:HD12	1:B:170:LEU:CG	1.93	0.98
1:A:610:TRP:CZ3	1:A:611:ASN:OD1	2.16	0.98
1:B:28:LYS:O	1:B:32:GLU:HG3	1.63	0.98
1:K:776:GLU:OE1	1:K:776:GLU:O	1.80	0.97
1:L:845:LEU:HD11	1:L:848:SER:CB	1.94	0.96
1:F:494:ASN:O	1:F:494:ASN:ND2	1.98	0.96
1:B:149:VAL:O	1:B:151:GLU:HG3	1.66	0.94
1:I:674:GLU:OE1	1:I:674:GLU:N	2.00	0.94
1:E:637:ARG:O	1:E:638:HIS:ND1	2.02	0.93
1:F:843:MET:CE	1:F:878:LEU:HD11	1.98	0.93
1:K:107:VAL:O	1:K:111:ILE:HD12	1.69	0.92
1:A:612:ILE:HD11	1:A:633:MET:SD	2.10	0.91
1:L:845:LEU:HD11	1:L:848:SER:OG	1.70	0.91
1:H:634:GLU:N	1:H:634:GLU:OE2	2.05	0.90
1:G:572:GLU:OE1	1:G:572:GLU:N	2.05	0.90
1:L:674:GLU:N	1:L:674:GLU:OE2	2.05	0.90
1:F:287:ASN:O	1:F:288:ARG:NH1	2.05	0.90
1:B:254:LEU:HD11	1:B:260:TYR:CD2	2.07	0.89
1:K:572:GLU:OE1	1:K:572:GLU:N	2.03	0.89
1:F:572:GLU:N	1:F:572:GLU:OE2	2.06	0.88
1:K:117:LYS:O	1:K:121:ILE:HD12	1.73	0.88
1:A:674:GLU:N	1:A:674:GLU:OE2	2.06	0.88
1:B:728:ILE:HG13	1:B:730:THR:HG23	1.56	0.88
1:F:841:GLN:HG2	1:F:875:ALA:O	1.73	0.88
1:L:27:VAL:HG21	1:L:111:ILE:HD11	1.55	0.88
1:K:103:ARG:HH11	1:K:107:VAL:HG13	1.37	0.87
1:D:674:GLU:N	1:D:674:GLU:OE1	2.07	0.87
1:F:841:GLN:NE2	1:F:874:ILE:HG21	1.89	0.87
1:B:237:GLN:OE1	1:B:238:TYR:CE1	2.27	0.87
1:B:572:GLU:N	1:B:572:GLU:OE2	2.08	0.87
1:F:612:ILE:HD11	1:F:633:MET:SD	2.15	0.87
1:E:572:GLU:OE1	1:E:572:GLU:N	2.07	0.86
1:I:151:GLU:HG3	1:I:152:GLU:HG3	1.57	0.86
1:J:637:ARG:O	1:J:638:HIS:ND1	2.08	0.86
1:J:572:GLU:OE1	1:J:572:GLU:N	2.08	0.86
1:F:103:ARG:HH11	1:F:107:VAL:HG23	1.39	0.86
1:K:606:MET:HE3	1:K:606:MET:O	1.76	0.86
1:F:354:VAL:HG21	3:F:902:ADP:H2'	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:VAL:O	1:G:10:VAL:HG23	1.76	0.85
1:E:612:ILE:HD11	1:E:633:MET:SD	2.17	0.85
1:I:637:ARG:O	1:I:638:HIS:ND1	2.10	0.85
1:D:437:GLN:OE1	1:D:437:GLN:N	2.09	0.84
1:G:151:GLU:HG3	1:G:152:GLU:HG3	1.59	0.84
1:B:584:TYR:OH	1:B:603:PRO:CG	2.26	0.84
1:A:82:ILE:O	1:A:86:LEU:HD22	1.77	0.84
1:L:151:GLU:HG3	1:L:152:GLU:HG3	1.59	0.84
1:L:82:ILE:O	1:L:86:LEU:HD23	1.77	0.84
1:B:155:VAL:HA	3:B:902:ADP:N6	1.92	0.84
1:K:637:ARG:O	1:K:638:HIS:ND1	2.11	0.84
1:I:277:LYS:HD2	1:I:277:LYS:O	1.78	0.83
1:B:165:VAL:HG11	1:B:196:ILE:HD13	1.61	0.83
1:E:503:SER:OG	1:E:504:GLU:OE1	1.96	0.83
1:K:103:ARG:HH11	1:K:107:VAL:CG1	1.91	0.83
1:K:67:ARG:HA	1:K:70:VAL:HG22	1.59	0.83
1:E:785:GLU:OE1	1:E:785:GLU:N	2.12	0.82
1:G:148:PRO:HB3	1:G:457:ASN:OD1	1.78	0.82
1:D:6:VAL:O	1:D:10:VAL:HG23	1.78	0.82
1:B:443:SER:HG	1:B:446:CYS:HG	1.27	0.82
1:C:175:HIS:HE1	1:C:177:GLU:HG2	1.42	0.82
1:L:6:VAL:O	1:L:10:VAL:HG23	1.79	0.82
1:E:114:ILE:O	1:E:118:VAL:HG23	1.79	0.82
1:G:785:GLU:N	1:G:785:GLU:OE1	2.13	0.82
1:J:29:GLU:OE1	1:J:29:GLU:N	2.12	0.82
1:K:732:LYS:NZ	1:K:780:SER:OG	2.13	0.81
1:G:173:SER:HA	1:G:286:PRO:HB3	1.63	0.81
1:J:165:VAL:HG11	1:J:196:ILE:HD13	1.61	0.81
1:C:175:HIS:CE1	1:C:177:GLU:HG2	2.15	0.81
1:E:714:LEU:HD12	1:E:717:LEU:HD12	1.61	0.81
1:L:148:PRO:HB3	1:L:457:ASN:OD1	1.80	0.81
1:H:277:LYS:O	1:H:277:LYS:NZ	2.11	0.81
1:G:329:ASP:OD1	1:G:330:LYS:N	2.15	0.80
1:K:157:GLY:O	1:K:310:LYS:NZ	2.14	0.80
1:A:151:GLU:HG3	1:A:152:GLU:HG3	1.62	0.80
1:F:637:ARG:O	1:F:638:HIS:ND1	2.14	0.80
1:B:612:ILE:HD11	1:B:633:MET:SD	2.22	0.80
1:F:521:ILE:HD12	1:F:525:VAL:HG23	1.62	0.80
1:L:832:ILE:HD11	1:L:862:LYS:HD3	1.61	0.80
1:D:572:GLU:N	1:D:572:GLU:OE1	2.14	0.79
1:G:21:VAL:O	1:G:25:SER:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:GLU:HG3	1:H:152:GLU:HG3	1.62	0.79
1:A:114:ILE:O	1:A:118:VAL:HG23	1.83	0.79
1:G:210:ILE:HD12	1:G:262:VAL:HG12	1.65	0.79
1:E:287:ASN:O	1:E:288:ARG:NH1	2.15	0.79
1:A:785:GLU:N	1:A:785:GLU:OE1	2.16	0.79
1:J:114:ILE:O	1:J:118:VAL:HG23	1.83	0.79
1:K:674:GLU:OE1	1:K:674:GLU:N	2.15	0.79
1:D:600:LYS:O	1:D:601:ILE:HD12	1.82	0.79
1:F:251:GLN:HG3	1:F:281:PRO:HB3	1.65	0.79
1:F:703:LYS:HE2	1:F:703:LYS:HA	1.64	0.79
1:L:785:GLU:N	1:L:785:GLU:OE1	2.16	0.79
1:B:785:GLU:OE1	1:B:785:GLU:N	2.16	0.78
1:B:782:GLU:OE1	1:B:782:GLU:N	2.16	0.78
1:J:785:GLU:OE2	1:J:785:GLU:N	2.16	0.78
1:J:287:ASN:O	1:J:288:ARG:NH1	2.16	0.78
1:A:838:ARG:NH2	1:A:866:GLN:OE1	2.16	0.78
1:D:146:LYS:O	1:D:148:PRO:HD3	1.84	0.78
1:E:782:GLU:OE1	1:E:782:GLU:N	2.17	0.78
1:I:550:GLU:OE1	1:I:550:GLU:N	2.17	0.78
1:E:845:LEU:HD11	1:E:848:SER:HB3	1.63	0.78
1:H:260:TYR:N	1:H:287:ASN:OD1	2.16	0.78
1:E:75:ASP:OD1	1:E:539:ARG:NH2	2.16	0.78
1:L:572:GLU:N	1:L:572:GLU:OE1	2.16	0.78
1:H:864:ASP:OD1	1:H:868:GLN:NE2	2.17	0.77
1:E:345:LYS:HZ3	1:E:378:SER:HB3	1.50	0.77
1:E:857:ARG:NH1	1:E:885:LEU:OXT	2.18	0.77
1:I:864:ASP:OD1	1:I:868:GLN:NE2	2.18	0.77
1:A:425:LYS:NZ	1:A:572:GLU:OE2	2.17	0.77
1:C:572:GLU:OE1	1:C:572:GLU:N	2.18	0.77
1:F:701:ASP:OD1	1:F:702:ASN:N	2.17	0.77
1:D:600:LYS:C	1:D:601:ILE:HD12	2.05	0.77
1:E:165:VAL:HG11	1:E:196:ILE:HD13	1.67	0.77
1:A:66:ILE:HD11	1:A:121:ILE:HG21	1.66	0.77
1:D:83:GLU:OE2	1:D:100:HIS:HE1	1.67	0.77
1:E:818:HIS:CE1	1:E:842:VAL:HG11	2.20	0.77
1:A:66:ILE:CD1	1:A:121:ILE:HG21	2.15	0.77
1:D:165:VAL:HG11	1:D:196:ILE:HD13	1.66	0.77
1:I:785:GLU:OE1	1:I:785:GLU:N	2.18	0.76
1:F:785:GLU:OE1	1:F:785:GLU:N	2.18	0.76
1:F:857:ARG:NH2	1:F:860:GLN:OE1	2.19	0.76
1:I:421:ILE:HD12	1:I:475:CYS:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:674:GLU:OE1	1:H:674:GLU:N	2.18	0.76
1:G:637:ARG:O	1:G:638:HIS:ND1	2.18	0.76
1:K:69:VAL:HG21	1:K:121:ILE:HD11	1.67	0.76
1:K:64:LYS:HZ2	1:K:65:LYS:H	1.33	0.76
1:F:103:ARG:NH1	1:F:107:VAL:HG23	2.01	0.76
1:H:785:GLU:OE1	1:H:785:GLU:N	2.17	0.76
1:J:702:ASN:OD1	1:J:703:LYS:N	2.18	0.76
1:B:287:ASN:O	1:B:288:ARG:NH1	2.18	0.76
1:J:829:GLU:OE1	1:J:829:GLU:N	2.18	0.76
1:L:169:LEU:HG	1:L:170:LEU:HG	1.68	0.76
1:D:860:GLN:NE2	1:D:864:ASP:OD2	2.19	0.76
1:G:35:LEU:O	1:G:39:ASN:ND2	2.18	0.76
1:I:582:GLU:N	1:I:582:GLU:OE1	2.19	0.76
1:D:175:HIS:O	1:D:288:ARG:NH2	2.19	0.75
1:D:785:GLU:N	1:D:785:GLU:OE1	2.18	0.75
1:A:254:LEU:HD11	1:A:260:TYR:CG	2.20	0.75
1:I:800:ARG:NH1	1:I:823:CYS:SG	2.59	0.75
1:A:108:ALA:HA	1:A:111:ILE:HD12	1.68	0.75
1:F:165:VAL:HG11	1:F:196:ILE:HD13	1.69	0.75
1:E:501:LEU:HD23	1:E:507:PHE:CE1	2.21	0.75
1:H:449:GLU:O	1:H:453:ASN:ND2	2.20	0.75
1:C:83:GLU:HG3	1:C:104:VAL:HG22	1.69	0.75
1:F:841:GLN:NE2	1:F:874:ILE:CG2	2.50	0.75
1:I:210:ILE:HG23	1:I:230:LYS:HE2	1.67	0.75
1:L:21:VAL:O	1:L:25:SER:N	2.20	0.75
1:A:767:GLU:OE1	1:A:767:GLU:N	2.21	0.74
1:D:29:GLU:OE1	1:D:29:GLU:N	2.18	0.74
1:H:582:GLU:OE1	1:H:582:GLU:N	2.20	0.74
1:I:37:ASP:OD2	1:I:122:ARG:NE	2.20	0.74
1:I:16:LEU:HD23	1:I:24:ILE:HD11	1.70	0.74
1:J:864:ASP:OD1	1:J:868:GLN:NE2	2.19	0.74
1:L:354:VAL:HG21	3:L:902:ADP:C8	2.22	0.74
1:E:254:LEU:HD21	1:E:260:TYR:CD2	2.21	0.74
1:H:443:SER:HG	1:H:446:CYS:HG	1.29	0.74
1:B:169:LEU:HD12	1:B:170:LEU:CD1	2.18	0.74
1:E:35:LEU:O	1:E:39:ASN:ND2	2.21	0.74
1:A:864:ASP:OD1	1:A:868:GLN:NE2	2.21	0.74
1:D:177:GLU:OE1	1:D:178:VAL:N	2.21	0.74
1:K:634:GLU:N	1:K:634:GLU:OE1	2.20	0.74
1:B:254:LEU:HD11	1:B:260:TYR:CB	2.16	0.74
1:K:785:GLU:OE1	1:K:785:GLU:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LEU:HD21	1:C:827:LEU:HD22	1.70	0.74
1:D:718:GLU:OE2	1:D:719:ASN:ND2	2.20	0.74
1:E:642:ASN:OD1	1:E:643:SER:N	2.21	0.74
1:E:724:ASN:HB3	1:E:752:ASP:HB3	1.70	0.74
1:D:234:ASN:ND2	1:D:237:GLN:OE1	2.21	0.74
1:G:846:GLN:HB2	1:G:881:PHE:CD2	2.22	0.74
1:L:29:GLU:OE1	1:L:29:GLU:N	2.21	0.73
1:A:443:SER:OG	1:A:446:CYS:SG	2.46	0.73
1:A:777:ASN:ND2	1:A:800:ARG:O	2.21	0.73
1:H:108:ALA:HA	1:H:111:ILE:HD12	1.70	0.73
1:G:175:HIS:O	1:G:288:ARG:NH2	2.22	0.73
1:L:177:GLU:OE1	1:L:178:VAL:N	2.22	0.73
1:I:178:VAL:HG22	1:I:289:VAL:HG22	1.68	0.73
1:E:148:PRO:HB3	1:E:457:ASN:OD1	1.88	0.73
1:D:637:ARG:O	1:D:638:HIS:ND1	2.22	0.73
1:I:99:PRO:O	1:I:100:HIS:ND1	2.21	0.73
1:A:857:ARG:NH2	1:A:885:LEU:O	2.22	0.73
1:C:820:VAL:CG1	1:C:822:ILE:HD11	2.19	0.73
1:K:733:LEU:HD12	1:K:753:THR:O	1.88	0.73
1:G:8:PHE:O	1:G:12:ASN:ND2	2.22	0.73
1:G:177:GLU:OE1	1:G:178:VAL:N	2.22	0.72
1:F:843:MET:HE3	1:F:878:LEU:HD11	1.70	0.72
1:I:777:ASN:ND2	1:I:800:ARG:O	2.22	0.72
1:K:151:GLU:HG3	1:K:152:GLU:HG3	1.69	0.72
1:C:329:ASP:OD1	1:C:330:LYS:N	2.22	0.72
1:D:829:GLU:N	1:D:829:GLU:OE1	2.22	0.72
1:I:220:ARG:NH2	1:I:275:ARG:O	2.22	0.72
1:B:149:VAL:O	1:B:151:GLU:CG	2.36	0.72
1:C:295:ASP:OD1	1:C:296:SER:N	2.21	0.72
1:F:157:GLY:O	1:F:310:LYS:NZ	2.22	0.72
1:F:634:GLU:OE1	1:F:634:GLU:N	2.23	0.72
1:K:172:GLU:OE2	1:K:175:HIS:HB3	1.90	0.72
1:L:845:LEU:CD1	1:L:848:SER:OG	2.37	0.72
1:D:445:GLU:OE1	1:D:445:GLU:N	2.21	0.72
1:I:287:ASN:O	1:I:288:ARG:NH1	2.23	0.72
1:J:262:VAL:CG2	1:J:289:VAL:HG22	2.20	0.72
1:L:480:MET:N	1:L:480:MET:SD	2.62	0.72
1:K:819:LEU:HD23	1:K:843:MET:CE	2.20	0.72
1:C:176:LEU:HB2	1:C:282:ASN:ND2	2.04	0.72
1:D:480:MET:N	1:D:480:MET:SD	2.63	0.72
1:A:582:GLU:N	1:A:582:GLU:OE1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:CD1	1:B:170:LEU:HG	2.12	0.71
1:D:163:ASP:OD1	1:D:164:ILE:N	2.23	0.71
1:H:198:LYS:HA	1:H:198:LYS:HE3	1.72	0.71
1:D:329:ASP:OD1	1:D:330:LYS:N	2.23	0.71
1:K:103:ARG:O	1:K:103:ARG:HD3	1.91	0.71
1:L:329:ASP:OD1	1:L:330:LYS:N	2.23	0.71
1:L:612:ILE:HD11	1:L:633:MET:SD	2.29	0.71
1:B:108:ALA:HA	1:B:111:ILE:HD12	1.72	0.71
1:B:584:TYR:OH	1:B:603:PRO:HG2	1.89	0.71
1:D:504:GLU:N	1:D:504:GLU:OE2	2.23	0.71
1:K:114:ILE:O	1:K:118:VAL:HG23	1.89	0.71
1:K:443:SER:HG	1:K:446:CYS:HG	1.35	0.71
1:I:315:ASP:OD1	1:I:316:GLU:N	2.23	0.71
1:I:829:GLU:N	1:I:829:GLU:OE1	2.24	0.71
1:J:536:GLU:OE1	1:J:536:GLU:N	2.23	0.71
1:L:445:GLU:OE1	1:L:445:GLU:N	2.23	0.71
1:K:449:GLU:O	1:K:453:ASN:ND2	2.24	0.71
1:L:637:ARG:O	1:L:638:HIS:ND1	2.23	0.71
1:A:702:ASN:HA	1:A:705:ALA:HB2	1.71	0.71
1:J:148:PRO:HB3	1:J:457:ASN:OD1	1.89	0.71
1:A:575:ASN:ND2	1:A:597:ASP:OD1	2.24	0.70
1:E:225:LEU:HD22	1:E:235:THR:HB	1.73	0.70
1:I:47:GLN:O	1:I:47:GLN:NE2	2.24	0.70
1:L:512:GLU:OE1	1:L:512:GLU:N	2.24	0.70
1:C:176:LEU:HD11	1:C:260:TYR:OH	1.90	0.70
1:L:843:MET:CE	1:L:878:LEU:HD13	2.21	0.70
1:C:211:TRP:CZ3	1:C:263:VAL:HG11	2.26	0.70
1:D:262:VAL:CG2	1:D:289:VAL:HG22	2.22	0.70
1:J:177:GLU:OE1	1:J:178:VAL:N	2.24	0.70
1:K:154:ASP:OD1	1:K:155:VAL:N	2.25	0.70
1:L:829:GLU:N	1:L:829:GLU:OE1	2.24	0.70
1:I:782:GLU:N	1:I:782:GLU:OE1	2.24	0.70
1:L:845:LEU:HD11	1:L:848:SER:HB2	1.73	0.70
1:D:612:ILE:HD11	1:D:633:MET:SD	2.31	0.70
1:G:64:LYS:C	1:G:65:LYS:HG3	2.10	0.70
1:K:714:LEU:HD12	1:K:717:LEU:HD12	1.73	0.70
1:C:785:GLU:OE1	1:C:785:GLU:N	2.24	0.70
1:C:151:GLU:HG3	1:C:152:GLU:HG3	1.74	0.70
1:E:262:VAL:CG2	1:E:289:VAL:HG22	2.21	0.70
1:I:425:LYS:NZ	1:I:572:GLU:OE2	2.25	0.70
1:L:100:HIS:ND1	1:L:100:HIS:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:O	1:A:288:ARG:NH1	2.24	0.70
1:E:82:ILE:CD1	1:E:565:LEU:CD2	2.69	0.70
1:G:582:GLU:OE1	1:G:582:GLU:N	2.25	0.70
1:G:612:ILE:HD11	1:G:633:MET:SD	2.32	0.70
1:K:59:LEU:HG	1:K:132:LEU:HD23	1.73	0.70
1:B:254:LEU:HD12	1:B:254:LEU:O	1.91	0.70
1:C:407:ALA:HB1	1:C:435:PHE:CD2	2.26	0.69
1:L:786:SER:O	1:L:807:LYS:NZ	2.24	0.69
1:A:207:PHE:CD1	1:A:207:PHE:O	2.44	0.69
1:C:151:GLU:HG2	1:C:327:HIS:HB3	1.74	0.69
1:D:84:ALA:O	1:D:88:LYS:HD2	1.91	0.69
1:H:120:GLU:O	1:H:124:THR:HG23	1.92	0.69
1:I:172:GLU:O	1:I:288:ARG:NH2	2.25	0.69
1:L:120:GLU:O	1:L:124:THR:HG23	1.92	0.69
1:K:119:ARG:NH1	1:K:119:ARG:O	2.24	0.69
1:E:845:LEU:HD11	1:E:848:SER:CB	2.23	0.69
1:F:16:LEU:HD23	1:F:24:ILE:HD11	1.74	0.69
1:G:751:LEU:HD23	1:G:776:GLU:OE1	1.93	0.69
1:H:287:ASN:O	1:H:288:ARG:NH1	2.24	0.69
1:B:835:ALA:O	1:B:863:LYS:NZ	2.23	0.69
1:A:28:LYS:NZ	1:A:32:GLU:OE2	2.24	0.69
1:A:169:LEU:CD1	1:A:170:LEU:HD23	2.22	0.69
1:B:96:LEU:HD22	1:B:101:TYR:CE2	2.27	0.69
1:B:169:LEU:CD1	1:B:170:LEU:CD1	2.70	0.69
1:E:408:CYS:O	1:E:411:TYR:N	2.26	0.69
1:G:221:ARG:NH2	1:G:239:HIS:O	2.26	0.69
1:I:27:VAL:O	1:I:27:VAL:HG22	1.93	0.69
1:B:262:VAL:CG2	1:B:289:VAL:HG22	2.23	0.69
1:C:120:GLU:O	1:C:124:THR:HG23	1.93	0.69
1:C:582:GLU:OE1	1:C:582:GLU:N	2.24	0.69
1:I:24:ILE:HG22	1:I:28:LYS:HA	1.72	0.69
1:E:344:LYS:O	1:E:344:LYS:NZ	2.17	0.68
1:G:715:GLU:OE1	1:G:715:GLU:N	2.24	0.68
1:H:708:LEU:O	1:H:708:LEU:HD12	1.92	0.68
1:F:437:GLN:OE1	1:F:437:GLN:N	2.25	0.68
1:G:413:SER:HB2	1:G:485:CYS:HB3	1.75	0.68
1:H:34:LEU:C	1:H:38:LEU:HD12	2.12	0.68
1:A:443:SER:HG	1:A:446:CYS:HG	1.36	0.68
1:D:169:LEU:HG	1:D:170:LEU:HD23	1.75	0.68
1:E:29:GLU:OE1	1:E:29:GLU:N	2.25	0.68
1:F:555:ASP:O	1:F:558:THR:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:GLU:O	1:I:124:THR:HG23	1.93	0.68
1:L:114:ILE:O	1:L:118:VAL:HG12	1.93	0.68
1:H:782:GLU:OE1	1:H:782:GLU:N	2.27	0.68
1:K:235:THR:O	1:K:239:HIS:ND1	2.25	0.68
1:J:163:ASP:OD1	1:J:164:ILE:N	2.26	0.68
1:A:34:LEU:HD21	1:A:73:ALA:HB1	1.76	0.68
1:A:782:GLU:N	1:A:782:GLU:OE1	2.27	0.68
1:C:504:GLU:OE1	1:C:504:GLU:N	2.26	0.68
1:D:166:ILE:HG12	1:D:202:ILE:HD11	1.76	0.68
1:G:119:ARG:NH2	1:G:123:GLN:OE1	2.24	0.68
1:E:174:ASN:ND2	1:E:284:ASN:O	2.26	0.68
1:I:130:GLN:OE1	1:I:130:GLN:N	2.27	0.68
1:I:271:GLU:OE2	1:I:275:ARG:NH2	2.27	0.68
1:D:96:LEU:HD22	1:D:101:TYR:CZ	2.29	0.68
1:G:443:SER:OG	1:G:446:CYS:SG	2.50	0.68
1:J:443:SER:OG	1:J:446:CYS:SG	2.51	0.68
1:B:603:PRO:O	1:B:628:ALA:HB2	1.94	0.68
1:E:741:PHE:HD2	1:E:766:LEU:HD11	1.59	0.68
1:G:210:ILE:HD12	1:G:262:VAL:CG1	2.24	0.68
1:I:21:VAL:O	1:I:25:SER:N	2.27	0.68
1:K:262:VAL:CG2	1:K:289:VAL:HG22	2.24	0.68
1:L:158:PHE:HE1	1:L:309:LEU:HD11	1.59	0.68
1:K:443:SER:OG	1:K:446:CYS:SG	2.51	0.67
1:L:175:HIS:O	1:L:288:ARG:NH2	2.27	0.67
1:J:44:PHE:CD1	1:J:132:LEU:HD11	2.29	0.67
1:L:41:PHE:HE2	1:L:118:VAL:HG23	1.59	0.67
1:B:155:VAL:HA	3:B:902:ADP:HN62	1.60	0.67
1:G:829:GLU:OE1	1:G:829:GLU:N	2.26	0.67
1:H:220:ARG:NH2	1:H:275:ARG:O	2.27	0.67
1:E:575:ASN:ND2	1:E:597:ASP:OD1	2.27	0.67
1:L:28:LYS:NZ	1:L:32:GLU:OE2	2.27	0.67
1:L:80:PHE:HE2	1:L:108:ALA:HB2	1.59	0.67
1:J:835:ALA:O	1:J:863:LYS:NZ	2.22	0.67
1:B:348:GLY:O	1:B:350:PRO:HD3	1.93	0.67
1:C:305:ILE:HG23	1:C:305:ILE:O	1.95	0.67
1:C:612:ILE:HD11	1:C:633:MET:SD	2.34	0.67
1:D:786:SER:O	1:D:807:LYS:NZ	2.25	0.67
1:F:262:VAL:CG2	1:F:289:VAL:HG22	2.24	0.67
1:F:427:ILE:O	1:F:431:ILE:HD12	1.95	0.67
1:C:35:LEU:O	1:C:39:ASN:ND2	2.28	0.67
1:G:480:MET:N	1:G:480:MET:SD	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:443:SER:OG	1:H:446:CYS:SG	2.44	0.67
1:H:829:GLU:OE1	1:H:829:GLU:N	2.27	0.67
1:F:58:VAL:O	1:F:62:LEU:HG	1.95	0.67
1:G:40:ASP:OD2	1:G:122:ARG:NH2	2.27	0.67
1:G:782:GLU:OE1	1:G:782:GLU:N	2.28	0.67
1:H:168:ARG:NH2	1:H:305:ILE:O	2.28	0.67
1:K:83:GLU:OE2	1:K:103:ARG:HD2	1.94	0.67
1:G:64:LYS:O	1:G:65:LYS:HG3	1.95	0.66
1:L:165:VAL:HG11	1:L:196:ILE:HD13	1.76	0.66
1:I:504:GLU:N	1:I:504:GLU:OE1	2.28	0.66
1:K:56:ASN:HD22	1:K:59:LEU:HD13	1.60	0.66
1:D:325:VAL:O	1:D:327:HIS:CE1	2.48	0.66
1:E:225:LEU:HD21	1:E:238:TYR:HB2	1.78	0.66
1:L:536:GLU:OE1	1:L:536:GLU:N	2.29	0.66
1:B:800:ARG:NH2	1:B:823:CYS:SG	2.68	0.66
1:D:83:GLU:OE1	1:D:100:HIS:CE1	2.48	0.66
1:I:566:LEU:HB2	1:I:586:LEU:HD22	1.77	0.66
1:I:757:TRP:CE2	1:I:803:LEU:HD13	2.30	0.66
1:L:809:SER:OG	1:L:811:ASP:OD1	2.13	0.66
1:C:755:LEU:O	1:C:780:SER:N	2.29	0.66
1:D:582:GLU:OE1	1:D:582:GLU:N	2.28	0.66
1:H:575:ASN:ND2	1:H:597:ASP:OD1	2.28	0.66
1:K:835:ALA:O	1:K:866:GLN:NE2	2.28	0.66
1:E:843:MET:CE	1:E:878:LEU:HD13	2.25	0.66
1:F:374:ASP:O	1:F:377:VAL:HG12	1.96	0.66
1:I:771:VAL:HG22	1:I:795:VAL:HG12	1.77	0.66
1:J:73:ALA:O	1:J:77:ILE:HG13	1.95	0.66
1:A:220:ARG:NH2	1:A:275:ARG:O	2.27	0.66
1:F:843:MET:HE2	1:F:878:LEU:CD1	2.26	0.66
1:K:56:ASN:HB3	1:K:59:LEU:HB2	1.76	0.66
1:C:752:ASP:N	1:C:776:GLU:OE1	2.29	0.66
1:E:254:LEU:HD22	1:E:281:PRO:HD2	1.77	0.66
1:F:591:TYR:HE1	1:F:593:ALA:HB2	1.61	0.66
1:H:643:SER:O	1:H:670:THR:OG1	2.14	0.66
1:L:369:GLU:O	1:L:373:VAL:HG23	1.96	0.66
1:F:818:HIS:NE2	1:F:820:VAL:HG23	2.11	0.65
1:K:410:LEU:HD12	1:K:489:ALA:HB2	1.78	0.65
1:F:10:VAL:O	1:F:14:MET:HG3	1.97	0.65
1:I:82:ILE:O	1:I:86:LEU:HD23	1.96	0.65
1:A:846:GLN:HB2	1:A:881:PHE:HD2	1.60	0.65
1:B:345:LYS:NZ	1:B:378:SER:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG11	1:C:196:ILE:HD13	1.78	0.65
1:D:369:GLU:O	1:D:373:VAL:HG23	1.96	0.65
1:G:262:VAL:HG23	1:G:289:VAL:HG22	1.77	0.65
1:J:169:LEU:HD12	1:J:170:LEU:HG	1.77	0.65
1:C:777:ASN:N	1:C:800:ARG:O	2.29	0.65
1:F:64:LYS:O	1:F:65:LYS:HB3	1.95	0.65
1:F:718:GLU:O	1:F:719:ASN:ND2	2.29	0.65
1:D:782:GLU:OE1	1:D:782:GLU:N	2.30	0.65
1:E:396:MET:O	1:E:400:ARG:NH1	2.29	0.65
1:L:110:GLU:O	1:L:114:ILE:HG13	1.97	0.65
1:C:369:GLU:O	1:C:373:VAL:HG23	1.96	0.65
1:H:501:LEU:HD11	1:H:507:PHE:CE1	2.32	0.65
1:H:592:VAL:O	1:H:592:VAL:HG13	1.96	0.65
1:I:592:VAL:HG13	1:I:592:VAL:O	1.96	0.65
1:L:305:ILE:HG23	1:L:305:ILE:O	1.97	0.65
1:G:74:GLU:O	1:G:78:ASP:OD1	2.15	0.65
1:F:526:LEU:HD11	1:F:552:PRO:HD3	1.78	0.65
1:G:215:SER:OG	1:G:216:GLN:N	2.30	0.65
1:H:639:LEU:O	1:H:639:LEU:HD23	1.97	0.65
1:E:121:ILE:O	1:E:125:ASP:N	2.28	0.64
1:A:725:ASP:OD1	1:A:726:SER:N	2.30	0.64
1:B:592:VAL:O	1:B:592:VAL:HG13	1.97	0.64
1:C:380:HIS:HB2	1:C:396:MET:HE1	1.78	0.64
1:D:443:SER:OG	1:D:446:CYS:SG	2.52	0.64
1:D:714:LEU:HD12	1:D:717:LEU:HD12	1.79	0.64
1:F:843:MET:CE	1:F:878:LEU:CD1	2.74	0.64
1:G:305:ILE:HG23	1:G:305:ILE:O	1.97	0.64
1:K:65:LYS:HA	1:K:68:THR:HG23	1.79	0.64
1:A:354:VAL:O	1:A:459:ASN:ND2	2.30	0.64
1:E:835:ALA:O	1:E:863:LYS:NZ	2.25	0.64
1:G:178:VAL:HG21	1:G:302:CYS:HB3	1.80	0.64
1:L:61:GLU:OE2	1:L:65:LYS:NZ	2.26	0.64
1:H:446:CYS:O	1:H:450:ASP:OD1	2.14	0.64
1:H:566:LEU:HB2	1:H:586:LEU:HD22	1.78	0.64
1:B:681:PHE:CD1	1:B:714:LEU:HD11	2.33	0.64
1:E:254:LEU:HD21	1:E:260:TYR:CE2	2.33	0.64
1:H:703:LYS:O	1:H:703:LYS:HD2	1.98	0.64
1:L:27:VAL:HG21	1:L:111:ILE:CD1	2.28	0.64
1:G:369:GLU:O	1:G:373:VAL:HG23	1.96	0.64
1:K:866:GLN:O	1:K:871:THR:OG1	2.15	0.64
1:A:103:ARG:HH11	1:A:106:GLU:HB3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:GLU:OE1	1:D:536:GLU:N	2.31	0.64
1:E:600:LYS:NZ	1:E:621:GLN:OE1	2.29	0.64
1:F:173:SER:HA	1:F:286:PRO:HB3	1.78	0.64
1:E:591:TYR:HE1	1:E:593:ALA:HB2	1.63	0.64
1:E:681:PHE:HD1	1:E:714:LEU:HD21	1.63	0.64
1:A:509:GLY:N	1:A:512:GLU:OE1	2.31	0.64
1:A:592:VAL:HG13	1:A:592:VAL:O	1.97	0.64
1:B:739:TYR:O	1:H:18:ARG:NH1	2.31	0.64
1:B:767:GLU:N	1:B:767:GLU:OE1	2.31	0.64
1:K:56:ASN:ND2	1:K:59:LEU:HD13	2.13	0.64
1:C:878:LEU:HD11	1:C:880:ILE:HG23	1.80	0.63
1:F:499:ILE:HD11	1:F:519:LEU:HD11	1.79	0.63
1:G:59:LEU:O	1:G:63:VAL:HG13	1.98	0.63
1:I:634:GLU:OE1	1:I:634:GLU:N	2.29	0.63
1:K:69:VAL:HG13	1:K:114:ILE:HD11	1.80	0.63
1:D:305:ILE:HG23	1:D:305:ILE:O	1.97	0.63
1:E:408:CYS:O	1:E:410:LEU:N	2.31	0.63
1:F:582:GLU:N	1:F:582:GLU:OE1	2.30	0.63
1:I:360:LEU:HD11	1:I:373:VAL:HG11	1.79	0.63
1:I:837:ILE:O	1:I:863:LYS:NZ	2.30	0.63
1:C:665:LEU:HD23	1:C:666:GLN:N	2.13	0.63
1:E:82:ILE:HG13	1:E:588:HIS:HE1	1.63	0.63
1:I:110:GLU:OE2	1:I:114:ILE:HD11	1.99	0.63
1:E:443:SER:HG	1:E:446:CYS:HG	1.46	0.63
1:J:767:GLU:OE1	1:J:767:GLU:N	2.31	0.63
1:K:177:GLU:OE1	1:K:178:VAL:N	2.30	0.63
1:L:262:VAL:CG2	1:L:289:VAL:HG22	2.29	0.63
1:L:582:GLU:OE1	1:L:582:GLU:N	2.30	0.63
1:B:877:LYS:HE3	1:B:879:SER:OG	1.98	0.63
1:L:163:ASP:OD1	1:L:164:ILE:N	2.31	0.63
1:C:490:MET:O	1:C:497:GLN:NE2	2.31	0.63
1:H:714:LEU:HD12	1:H:717:LEU:HD12	1.79	0.63
1:J:800:ARG:NH2	1:J:823:CYS:SG	2.71	0.63
1:K:82:ILE:O	1:K:86:LEU:HD23	1.99	0.63
1:I:82:ILE:HG13	1:I:588:HIS:CE1	2.33	0.63
1:I:671:ILE:HD11	1:I:675:SER:O	1.98	0.63
1:B:409:PHE:CE1	1:B:477:LEU:HD21	2.33	0.63
1:G:29:GLU:OE1	1:G:29:GLU:N	2.31	0.63
1:E:117:LYS:O	1:E:121:ILE:HD12	1.99	0.63
1:H:692:ILE:HD13	1:H:699:LEU:HD11	1.81	0.63
1:J:443:SER:HG	1:J:446:CYS:HG	1.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:501:LEU:HD11	1:J:507:PHE:CE1	2.34	0.63
1:C:692:ILE:HD13	1:C:699:LEU:HD11	1.80	0.62
1:F:788:GLY:N	1:F:812:ASP:OD1	2.32	0.62
1:H:146:LYS:HB3	1:H:147:PRO:HD2	1.81	0.62
1:E:665:LEU:HD23	1:E:666:GLN:N	2.14	0.62
1:K:23:LEU:HD12	1:K:81:VAL:HG13	1.81	0.62
1:L:34:LEU:CD1	1:L:118:VAL:HG11	2.28	0.62
1:B:221:ARG:NH2	1:B:239:HIS:O	2.32	0.62
1:D:471:GLN:OE1	1:D:471:GLN:N	2.33	0.62
1:I:178:VAL:HG22	1:I:289:VAL:CG2	2.28	0.62
1:A:671:ILE:HD11	1:A:675:SER:O	2.00	0.62
1:E:767:GLU:N	1:E:767:GLU:OE1	2.32	0.62
1:I:291:LEU:C	1:I:291:LEU:HD12	2.20	0.62
1:J:714:LEU:HD12	1:J:717:LEU:HD12	1.82	0.62
1:I:148:PRO:HG3	1:I:453:ASN:HB3	1.82	0.62
1:K:67:ARG:HA	1:K:70:VAL:CG2	2.29	0.62
1:E:725:ASP:OD1	1:E:726:SER:N	2.33	0.62
1:I:229:SER:O	1:I:233:ARG:NH2	2.31	0.62
1:L:27:VAL:O	1:L:27:VAL:HG22	2.00	0.62
1:A:103:ARG:O	1:A:107:VAL:HG23	1.99	0.62
1:B:274:GLU:OE1	1:B:277:LYS:NZ	2.20	0.62
1:B:584:TYR:CD2	1:B:605:LEU:HB2	2.34	0.62
1:C:27:VAL:HG21	1:C:111:ILE:CD1	2.29	0.62
1:J:647:LEU:HD11	1:J:668:LEU:HD13	1.82	0.62
1:K:413:SER:HB3	1:K:485:CYS:HB2	1.82	0.62
1:B:3:ASN:O	1:B:7:GLU:HG3	1.99	0.62
1:J:217:SER:O	1:J:217:SER:OG	2.18	0.62
1:K:186:GLY:HA3	1:K:351:LEU:HD22	1.81	0.62
1:A:146:LYS:HB3	1:A:147:PRO:HD2	1.81	0.61
1:B:501:LEU:HD21	1:B:507:PHE:CE1	2.34	0.61
1:C:174:ASN:HA	1:C:284:ASN:C	2.19	0.61
1:C:27:VAL:HG11	1:C:111:ILE:CD1	2.30	0.61
1:L:782:GLU:OE1	1:L:782:GLU:N	2.33	0.61
1:A:566:LEU:HB2	1:A:586:LEU:HD22	1.83	0.61
1:K:463:VAL:HG22	1:K:472:ILE:HD11	1.81	0.61
1:C:829:GLU:OE1	1:C:829:GLU:N	2.33	0.61
1:D:136:ASP:OD1	1:D:137:LEU:N	2.33	0.61
1:E:412:CYS:HB3	1:E:477:LEU:HD11	1.83	0.61
1:I:146:LYS:HB3	1:I:147:PRO:HD2	1.82	0.61
1:I:210:ILE:HD12	1:I:230:LYS:HE2	1.82	0.61
1:L:178:VAL:HG21	1:L:302:CYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:555:ASP:O	1:L:558:THR:OG1	2.16	0.61
1:A:178:VAL:HG12	1:A:289:VAL:CG2	2.30	0.61
1:A:360:LEU:HD11	1:A:373:VAL:HG11	1.83	0.61
1:C:151:GLU:HG3	1:C:152:GLU:OE2	2.00	0.61
1:D:176:LEU:HD11	1:D:260:TYR:OH	2.00	0.61
1:E:136:ASP:OD1	1:E:137:LEU:N	2.32	0.61
1:I:82:ILE:HD12	1:I:565:LEU:CD2	2.30	0.61
1:J:52:HIS:ND1	1:J:52:HIS:O	2.32	0.61
1:A:27:VAL:O	1:A:27:VAL:HG22	2.01	0.61
1:A:647:LEU:CD1	1:A:671:ILE:HD12	2.31	0.61
1:H:96:LEU:HD13	1:H:101:TYR:CD2	2.36	0.61
1:H:767:GLU:N	1:H:767:GLU:OE1	2.33	0.61
1:I:501:LEU:HD11	1:I:507:PHE:CE1	2.36	0.61
1:K:800:ARG:NH1	1:K:823:CYS:SG	2.73	0.61
1:L:155:VAL:HG13	3:L:902:ADP:N6	2.16	0.61
1:L:215:SER:OG	1:L:216:GLN:N	2.34	0.61
1:L:630:ILE:HD11	1:L:647:LEU:CD1	2.30	0.61
1:A:169:LEU:HD12	1:A:170:LEU:HB2	1.82	0.61
1:A:175:HIS:O	1:A:288:ARG:NH1	2.34	0.61
1:E:401:LEU:HD21	1:E:405:LEU:HB3	1.83	0.61
1:H:725:ASP:OD1	1:H:726:SER:N	2.34	0.61
1:K:591:TYR:HE1	1:K:593:ALA:HB2	1.65	0.61
1:C:224:PHE:CZ	1:C:279:ALA:HB2	2.35	0.61
1:H:208:THR:OG1	1:H:259:LYS:O	2.19	0.61
1:I:725:ASP:OD1	1:I:726:SER:N	2.34	0.61
1:J:555:ASP:O	1:J:558:THR:HG22	2.01	0.61
1:C:393:LEU:HD23	1:C:396:MET:HE3	1.83	0.61
1:D:215:SER:OG	1:D:216:GLN:N	2.31	0.61
1:A:216:GLN:OE1	1:A:216:GLN:O	2.19	0.60
1:B:369:GLU:O	1:B:373:VAL:HG23	2.01	0.60
1:D:54:ASN:O	1:D:60:ARG:NH2	2.33	0.60
1:F:592:VAL:HG23	1:F:592:VAL:O	2.01	0.60
1:I:409:PHE:O	1:I:412:CYS:SG	2.59	0.60
1:L:864:ASP:OD1	1:L:868:GLN:NE2	2.34	0.60
1:D:69:VAL:CG1	1:D:118:VAL:HG12	2.31	0.60
1:D:752:ASP:OD1	1:D:754:TRP:NE1	2.32	0.60
1:E:21:VAL:O	1:E:25:SER:N	2.34	0.60
1:F:120:GLU:O	1:F:124:THR:HG23	2.00	0.60
1:L:843:MET:HE3	1:L:878:LEU:HD13	1.82	0.60
1:A:178:VAL:HG12	1:A:289:VAL:HG22	1.83	0.60
1:E:592:VAL:O	1:E:592:VAL:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:818:HIS:ND1	1:E:842:VAL:HG11	2.15	0.60
1:A:207:PHE:O	1:A:207:PHE:HD1	1.84	0.60
1:B:584:TYR:OH	1:B:603:PRO:CB	2.49	0.60
1:F:65:LYS:HD2	1:F:68:THR:OG1	2.00	0.60
1:K:376:SER:OG	1:K:396:MET:SD	2.57	0.60
1:L:27:VAL:HG11	1:L:111:ILE:HD11	1.84	0.60
1:L:146:LYS:HB3	1:L:147:PRO:HD2	1.83	0.60
1:H:114:ILE:O	1:H:118:VAL:HG23	2.01	0.60
1:K:59:LEU:HG	1:K:132:LEU:HB3	1.82	0.60
1:F:758:LYS:NZ	1:F:785:GLU:OE2	2.28	0.60
1:K:59:LEU:HG	1:K:132:LEU:CD2	2.32	0.60
1:A:169:LEU:HD12	1:A:170:LEU:HD23	1.84	0.60
1:B:226:ASN:OD1	1:B:227:ILE:N	2.35	0.60
1:B:402:PRO:HD2	1:B:405:LEU:HD12	1.84	0.60
1:B:488:GLU:OE1	1:B:488:GLU:C	2.40	0.60
1:E:345:LYS:NZ	1:E:378:SER:HB3	2.15	0.60
1:G:350:PRO:O	1:G:354:VAL:HG23	2.02	0.60
1:G:136:ASP:OD1	1:G:137:LEU:N	2.35	0.60
1:I:82:ILE:HG13	1:I:588:HIS:HE1	1.66	0.60
1:E:369:GLU:O	1:E:373:VAL:HG23	2.00	0.60
1:J:100:HIS:O	1:J:105:LYS:NZ	2.27	0.60
1:B:334:GLU:OE1	1:B:334:GLU:N	2.33	0.60
1:E:217:SER:OG	1:E:217:SER:O	2.20	0.60
1:A:11:GLU:OE1	1:A:437:GLN:NE2	2.32	0.59
1:E:800:ARG:NH1	1:E:823:CYS:SG	2.75	0.59
1:G:464:MET:CE	1:G:476:ARG:HD3	2.32	0.59
1:H:408:CYS:HG	1:H:430:TRP:HZ2	1.47	0.59
1:J:823:CYS:N	1:J:846:GLN:OE1	2.31	0.59
1:J:582:GLU:OE1	1:J:582:GLU:N	2.36	0.59
1:B:345:LYS:HZ3	1:B:378:SER:HB3	1.67	0.59
1:E:714:LEU:CD1	1:E:717:LEU:HD12	2.31	0.59
1:A:216:GLN:O	1:A:216:GLN:CD	2.40	0.59
1:C:820:VAL:HG22	1:C:844:MET:HB3	1.85	0.59
1:F:463:VAL:HG13	1:F:472:ILE:HG23	1.82	0.59
1:I:265:ASP:OD1	1:I:292:THR:OG1	2.16	0.59
1:K:69:VAL:HG21	1:K:121:ILE:CD1	2.31	0.59
1:A:757:TRP:CE2	1:A:803:LEU:HD13	2.36	0.59
1:B:52:HIS:ND1	1:B:52:HIS:O	2.34	0.59
1:C:210:ILE:HB	1:C:262:VAL:HG12	1.84	0.59
1:F:643:SER:OG	1:F:644:SER:N	2.33	0.59
1:H:757:TRP:CE2	1:H:803:LEU:HD13	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:592:VAL:O	1:J:592:VAL:HG13	2.02	0.59
1:K:416:PRO:HD3	1:K:544:PHE:CD2	2.37	0.59
1:D:21:VAL:O	1:D:25:SER:N	2.36	0.59
1:D:83:GLU:CD	1:D:100:HIS:CE1	2.76	0.59
1:E:734:ARG:NH1	1:E:759:ASP:OD1	2.35	0.59
1:I:835:ALA:HB2	1:I:859:ILE:HG23	1.85	0.59
1:I:169:LEU:C	1:I:170:LEU:HD12	2.23	0.59
1:H:27:VAL:O	1:H:27:VAL:HG22	2.02	0.59
1:D:83:GLU:OE2	1:D:100:HIS:CE1	2.54	0.59
1:E:408:CYS:O	1:E:409:PHE:C	2.41	0.59
1:I:575:ASN:ND2	1:I:597:ASP:OD1	2.36	0.59
1:K:173:SER:HA	1:K:286:PRO:HB3	1.84	0.59
1:D:696:ILE:HG22	1:D:700:LEU:HD23	1.85	0.58
1:D:816:LEU:HD23	1:D:817:LYS:N	2.18	0.58
1:F:356:ILE:HD11	1:F:393:LEU:HD21	1.84	0.58
1:H:434:GLY:O	1:H:437:GLN:NE2	2.36	0.58
1:H:752:ASP:N	1:H:776:GLU:OE1	2.36	0.58
1:B:172:GLU:O	1:B:288:ARG:NH2	2.36	0.58
1:E:696:ILE:HG22	1:E:700:LEU:HD23	1.84	0.58
1:F:354:VAL:HG21	3:F:902:ADP:C2'	2.32	0.58
1:I:847:ASN:ND2	1:I:847:ASN:O	2.34	0.58
1:J:591:TYR:HE1	1:J:593:ALA:HB2	1.68	0.58
1:L:58:VAL:O	1:L:62:LEU:HG	2.04	0.58
1:A:401:LEU:HD12	1:A:458:ARG:NH1	2.17	0.58
1:B:79:LYS:NZ	1:B:536:GLU:OE2	2.35	0.58
1:D:96:LEU:HD22	1:D:101:TYR:CE1	2.38	0.58
1:E:192:LEU:HD11	1:E:196:ILE:HD11	1.86	0.58
1:F:154:ASP:OD1	1:F:155:VAL:N	2.36	0.58
1:G:83:GLU:OE1	1:G:104:VAL:HG23	2.03	0.58
1:K:60:ARG:O	1:K:63:VAL:HG22	2.04	0.58
1:L:773:LYS:NZ	2:L:901:IHP:O25	2.37	0.58
1:C:176:LEU:HD22	1:C:287:ASN:HB2	1.85	0.58
1:K:115:ARG:HD2	1:K:115:ARG:O	2.03	0.58
1:K:360:LEU:HD23	1:K:373:VAL:HG21	1.85	0.58
1:L:125:ASP:OD1	1:L:125:ASP:N	2.37	0.58
1:B:178:VAL:HG12	1:B:289:VAL:HB	1.85	0.58
1:F:774:MET:HG2	1:F:798:ILE:HD12	1.84	0.58
1:I:350:PRO:CB	3:I:902:ADP:C8	2.87	0.58
1:E:34:LEU:HD23	1:E:118:VAL:HG21	1.86	0.58
1:F:645:ALA:O	1:F:672:ALA:N	2.37	0.58
1:K:166:ILE:HG23	1:K:202:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:SER:HA	1:D:286:PRO:HB3	1.85	0.58
1:E:120:GLU:OE2	1:E:121:ILE:N	2.35	0.58
1:F:360:LEU:HD23	1:F:373:VAL:HG21	1.85	0.58
1:J:262:VAL:HG23	1:J:289:VAL:HG22	1.84	0.58
1:L:98:LEU:HB2	1:L:99:PRO:HD3	1.85	0.58
1:L:843:MET:HE2	1:L:878:LEU:HD13	1.85	0.58
1:A:846:GLN:HB2	1:A:881:PHE:CD2	2.39	0.58
1:J:334:GLU:OE1	1:J:334:GLU:N	2.33	0.58
1:B:443:SER:OG	1:B:446:CYS:SG	2.50	0.58
1:C:192:LEU:HD11	1:C:196:ILE:HD11	1.86	0.58
1:C:480:MET:N	1:C:480:MET:SD	2.77	0.58
1:E:816:LEU:HD23	1:E:817:LYS:N	2.19	0.58
1:G:168:ARG:HH21	1:G:179:VAL:HG13	1.68	0.58
1:G:223:LEU:CD2	1:G:276:ILE:HD11	2.34	0.58
1:G:464:MET:HE1	1:G:476:ARG:HD3	1.85	0.58
1:J:816:LEU:HD23	1:J:817:LYS:N	2.18	0.58
1:K:41:PHE:O	1:K:45:LEU:HG	2.02	0.58
1:K:67:ARG:CA	1:K:70:VAL:HG22	2.33	0.58
1:A:735:LEU:HD13	1:A:763:LEU:HD21	1.86	0.58
1:B:148:PRO:HG2	1:B:457:ASN:ND2	2.19	0.58
1:D:74:GLU:O	1:D:78:ASP:OD2	2.22	0.58
1:G:718:GLU:N	1:G:718:GLU:OE2	2.36	0.58
1:B:192:LEU:HD11	1:B:196:ILE:HD11	1.86	0.57
1:B:254:LEU:CD1	1:B:260:TYR:CD2	2.83	0.57
1:E:207:PHE:CD1	1:E:883:PRO:HD3	2.39	0.57
1:A:714:LEU:HD12	1:A:717:LEU:HD12	1.87	0.57
1:B:437:GLN:H	1:B:439:LYS:NZ	2.01	0.57
1:F:521:ILE:CD1	1:F:525:VAL:HG23	2.32	0.57
1:H:169:LEU:O	1:H:170:LEU:HG	2.04	0.57
1:K:111:ILE:HA	1:K:114:ILE:HG22	1.86	0.57
1:K:643:SER:OG	1:K:644:SER:N	2.37	0.57
1:A:643:SER:O	1:A:670:THR:OG1	2.21	0.57
1:B:408:CYS:HB3	1:B:430:TRP:CZ2	2.39	0.57
1:D:555:ASP:O	1:D:558:THR:OG1	2.17	0.57
1:H:34:LEU:O	1:H:38:LEU:CD1	2.34	0.57
1:J:820:VAL:HG13	1:J:844:MET:HE3	1.86	0.57
1:L:832:ILE:HD11	1:L:862:LYS:CD	2.31	0.57
1:B:217:SER:O	1:B:217:SER:OG	2.17	0.57
1:D:777:ASN:N	1:D:800:ARG:O	2.37	0.57
1:E:82:ILE:HG13	1:E:588:HIS:CE1	2.39	0.57
1:E:818:HIS:ND1	1:E:842:VAL:CG1	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:SER:HB3	1:F:485:CYS:HB2	1.86	0.57
1:K:176:LEU:HA	1:K:287:ASN:O	2.04	0.57
1:D:83:GLU:CD	1:D:100:HIS:HE1	2.06	0.57
1:I:612:ILE:HD11	1:I:633:MET:SD	2.44	0.57
1:J:360:LEU:HD21	1:J:373:VAL:HG11	1.85	0.57
1:J:610:TRP:NE1	1:J:611:ASN:OD1	2.37	0.57
1:J:880:ILE:HD11	1:J:885:LEU:HB2	1.87	0.57
1:K:166:ILE:HA	1:K:169:LEU:HD11	1.85	0.57
1:A:219:ARG:HD2	1:A:222:GLU:OE2	2.05	0.57
1:E:670:THR:HG21	1:E:693:ARG:HE	1.70	0.57
1:F:494:ASN:HD22	1:F:494:ASN:C	2.02	0.57
1:H:160:GLU:OE2	1:H:310:LYS:NZ	2.31	0.57
1:J:233:ARG:HA	1:J:233:ARG:NE	2.19	0.57
1:D:178:VAL:HG21	1:D:302:CYS:HB3	1.86	0.57
1:D:408:CYS:SG	1:D:455:LEU:HD13	2.45	0.57
1:E:429:LEU:HD23	1:E:591:TYR:CE2	2.39	0.57
1:G:262:VAL:CG2	1:G:289:VAL:HG22	2.34	0.57
1:K:37:ASP:O	1:K:41:PHE:CD2	2.58	0.57
1:K:103:ARG:NH1	1:K:107:VAL:CG1	2.64	0.57
1:K:651:VAL:O	1:K:651:VAL:HG13	2.05	0.57
1:K:819:LEU:HD23	1:K:843:MET:HE3	1.86	0.57
1:D:449:GLU:OE1	1:D:449:GLU:O	2.23	0.57
1:E:151:GLU:HG3	1:E:152:GLU:HG3	1.87	0.57
1:G:146:LYS:HB3	1:G:147:PRO:HD2	1.85	0.57
1:G:708:LEU:HD23	1:G:736:PRO:HG3	1.86	0.57
1:I:255:GLY:O	1:I:285:LYS:NZ	2.37	0.57
1:I:771:VAL:HG22	1:I:795:VAL:CG1	2.35	0.57
1:J:107:VAL:HG13	1:J:107:VAL:O	2.03	0.57
1:B:82:ILE:O	1:B:86:LEU:HD13	2.04	0.57
1:F:169:LEU:HG	1:F:170:LEU:HG	1.86	0.57
1:H:701:ASP:OD1	1:H:702:ASN:N	2.38	0.57
1:I:159:ASP:OD1	1:I:160:GLU:N	2.37	0.57
1:L:755:LEU:O	1:L:780:SER:N	2.38	0.57
1:C:633:MET:O	1:C:662:ASN:ND2	2.38	0.57
1:E:695:LYS:O	1:E:698:VAL:HG12	2.05	0.57
1:F:841:GLN:HE21	1:F:874:ILE:HB	1.69	0.57
1:F:843:MET:HE1	1:F:856:ALA:HB1	1.86	0.57
1:G:192:LEU:HD11	1:G:196:ILE:HD11	1.87	0.57
1:C:421:ILE:HG21	1:C:426:LEU:HD21	1.86	0.56
1:G:120:GLU:O	1:G:124:THR:HG23	2.05	0.56
1:I:350:PRO:HB2	3:I:902:ADP:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:752:ASP:OD1	1:J:754:TRP:NE1	2.38	0.56
1:L:750:LEU:CD2	1:L:753:THR:HG21	2.34	0.56
1:C:809:SER:OG	1:C:811:ASP:OD1	2.23	0.56
1:G:797:TRP:CD2	1:G:820:VAL:HG11	2.40	0.56
1:I:277:LYS:HD2	1:I:277:LYS:C	2.26	0.56
1:J:734:ARG:NH1	1:J:759:ASP:OD1	2.37	0.56
1:A:120:GLU:O	1:A:124:THR:HG23	2.05	0.56
1:A:265:ASP:OD1	1:A:292:THR:OG1	2.22	0.56
1:B:132:LEU:HD12	1:B:133:GLN:N	2.21	0.56
1:D:41:PHE:O	1:D:45:LEU:HG	2.05	0.56
1:E:325:VAL:O	1:E:361:ILE:HD11	2.06	0.56
1:F:215:SER:OG	1:F:216:GLN:N	2.39	0.56
1:H:464:MET:HE1	1:H:476:ARG:HD3	1.86	0.56
1:I:233:ARG:NE	1:I:233:ARG:HA	2.20	0.56
1:J:725:ASP:OD1	1:J:726:SER:N	2.38	0.56
1:K:64:LYS:NZ	1:K:65:LYS:H	2.01	0.56
1:L:843:MET:CE	1:L:878:LEU:HD22	2.34	0.56
1:F:665:LEU:HD23	1:F:666:GLN:N	2.20	0.56
1:H:103:ARG:O	1:H:107:VAL:HG23	2.05	0.56
1:K:58:VAL:O	1:K:62:LEU:HG	2.05	0.56
1:L:100:HIS:HD1	1:L:104:VAL:HG23	1.71	0.56
1:B:92:VAL:HG11	1:B:97:ASP:CG	2.25	0.56
1:E:315:ASP:OD1	1:E:316:GLU:N	2.38	0.56
1:F:703:LYS:O	1:F:703:LYS:HD3	2.06	0.56
1:L:173:SER:HA	1:L:286:PRO:HB3	1.85	0.56
1:B:331:CYS:SG	1:B:336:VAL:HG22	2.46	0.56
1:E:169:LEU:C	1:E:170:LEU:HD12	2.26	0.56
1:F:66:ILE:O	1:F:69:VAL:HG12	2.06	0.56
1:H:464:MET:CE	1:H:476:ARG:HD3	2.35	0.56
1:I:776:GLU:N	1:I:799:GLU:OE2	2.34	0.56
1:J:208:THR:OG1	1:J:259:LYS:O	2.23	0.56
1:J:612:ILE:HD11	1:J:633:MET:SD	2.45	0.56
1:J:702:ASN:OD1	1:J:702:ASN:C	2.44	0.56
1:K:498:GLU:OE2	1:K:522:HIS:ND1	2.35	0.56
1:K:555:ASP:O	1:K:558:THR:HG22	2.06	0.56
1:L:74:GLU:O	1:L:78:ASP:OD2	2.24	0.56
1:A:327:HIS:N	1:A:327:HIS:CD2	2.74	0.56
1:A:345:LYS:O	1:A:381:LEU:HD23	2.06	0.56
1:A:639:LEU:O	1:A:639:LEU:HD23	2.06	0.56
1:C:215:SER:OG	1:C:216:GLN:N	2.39	0.56
1:G:449:GLU:OE2	1:G:449:GLU:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:ARG:HD2	1:I:222:GLU:OE2	2.05	0.56
1:A:27:VAL:HG21	1:A:111:ILE:HG21	1.88	0.56
1:A:172:GLU:HG3	1:A:172:GLU:O	2.06	0.56
1:A:610:TRP:CE3	1:A:611:ASN:OD1	2.58	0.56
1:C:100:HIS:O	1:C:104:VAL:HG23	2.06	0.56
1:F:841:GLN:CD	1:F:874:ILE:CG2	2.73	0.56
1:G:74:GLU:O	1:G:77:ILE:HG22	2.06	0.56
1:J:314:GLU:OE1	1:J:344:LYS:HA	2.06	0.56
1:J:701:ASP:OD2	1:J:703:LYS:NZ	2.35	0.56
1:K:14:MET:HG2	1:K:35:LEU:HD11	1.87	0.56
1:K:829:GLU:OE1	1:K:829:GLU:N	2.38	0.56
1:L:816:LEU:HD23	1:L:817:LYS:N	2.21	0.56
1:A:148:PRO:HB3	1:A:457:ASN:OD1	2.06	0.55
1:I:172:GLU:HB2	1:I:175:HIS:CE1	2.42	0.55
1:I:172:GLU:HB2	1:I:175:HIS:ND1	2.20	0.55
1:I:197:TYR:O	1:I:209:ARG:NH1	2.39	0.55
1:C:392:LYS:O	1:C:396:MET:HG3	2.07	0.55
1:H:700:LEU:HD12	1:H:734:ARG:O	2.06	0.55
1:J:429:LEU:HD23	1:J:591:TYR:CE2	2.41	0.55
1:K:271:GLU:OE1	1:K:271:GLU:N	2.39	0.55
1:A:207:PHE:CD1	1:A:207:PHE:C	2.78	0.55
1:B:24:ILE:O	1:B:24:ILE:HG22	2.06	0.55
1:E:818:HIS:CE1	1:E:842:VAL:CG1	2.89	0.55
1:F:612:ILE:HD12	1:F:615:ILE:HD11	1.87	0.55
1:F:639:LEU:O	1:F:639:LEU:HD23	2.05	0.55
1:H:36:GLN:O	1:H:40:ASP:OD1	2.24	0.55
1:H:100:HIS:O	1:H:104:VAL:HG23	2.06	0.55
1:H:260:TYR:OH	1:H:281:PRO:O	2.23	0.55
1:H:624:LEU:HD12	1:H:625:ASP:N	2.22	0.55
1:F:148:PRO:HG3	1:F:457:ASN:OD1	2.07	0.55
1:F:819:LEU:O	1:F:843:MET:HA	2.07	0.55
1:K:494:ASN:O	1:K:494:ASN:ND2	2.39	0.55
1:A:128:GLY:C	1:A:129:LEU:HD23	2.27	0.55
1:B:734:ARG:NH1	1:B:759:ASP:OD1	2.39	0.55
1:G:445:GLU:OE1	1:G:445:GLU:N	2.36	0.55
1:K:575:ASN:ND2	1:K:597:ASP:OD1	2.39	0.55
1:L:262:VAL:HG23	1:L:289:VAL:HG22	1.88	0.55
1:L:443:SER:OG	1:L:446:CYS:SG	2.56	0.55
1:L:752:ASP:OD1	1:L:754:TRP:NE1	2.37	0.55
1:E:700:LEU:HD12	1:E:734:ARG:O	2.06	0.55
1:B:16:LEU:HD21	1:B:81:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:GLU:OE1	1:B:489:ALA:N	2.40	0.55
1:C:164:ILE:O	1:C:168:ARG:HG2	2.06	0.55
1:C:263:VAL:HG22	1:C:290:LEU:HB3	1.88	0.55
1:D:84:ALA:O	1:D:88:LYS:CD	2.55	0.55
1:F:103:ARG:O	1:F:103:ARG:HD3	2.06	0.55
1:G:30:ALA:O	1:G:34:LEU:HG	2.07	0.55
1:G:110:GLU:OE1	1:G:110:GLU:HA	2.06	0.55
1:I:190:THR:HG22	3:I:902:ADP:O3A	2.07	0.55
1:I:639:LEU:O	1:I:639:LEU:HD23	2.07	0.55
1:K:165:VAL:HG11	1:K:196:ILE:HD13	1.89	0.55
1:E:34:LEU:CD2	1:E:118:VAL:HG21	2.36	0.55
1:I:232:THR:O	1:I:233:ARG:NH2	2.39	0.55
1:I:800:ARG:NH2	1:I:825:ASP:OD1	2.37	0.55
1:A:225:LEU:CD2	1:A:246:LEU:HD11	2.37	0.55
1:C:428:ARG:HH21	1:C:638:HIS:CE1	2.25	0.55
1:D:350:PRO:O	1:D:354:VAL:HG23	2.06	0.55
1:E:154:ASP:OD1	1:E:154:ASP:N	2.40	0.55
1:F:735:LEU:CD1	1:F:763:LEU:HD21	2.36	0.55
1:F:818:HIS:NE2	1:F:820:VAL:CG2	2.70	0.55
1:J:315:ASP:OD1	1:J:316:GLU:N	2.40	0.55
1:A:692:ILE:HD13	1:A:699:LEU:HD11	1.88	0.55
1:B:591:TYR:HE1	1:B:593:ALA:HB2	1.72	0.55
1:G:777:ASN:N	1:G:800:ARG:O	2.39	0.55
1:H:80:PHE:O	1:H:80:PHE:HD1	1.90	0.55
1:J:154:ASP:N	1:J:154:ASP:OD1	2.40	0.55
1:J:224:PHE:O	1:J:228:ILE:HG22	2.07	0.55
1:J:735:LEU:CD1	1:J:763:LEU:HD21	2.37	0.55
1:K:433:GLU:CD	1:K:568:VAL:HG21	2.28	0.55
1:L:777:ASN:N	1:L:800:ARG:O	2.39	0.55
1:A:66:ILE:HD11	1:A:121:ILE:CG2	2.35	0.54
1:A:197:TYR:O	1:A:209:ARG:NH1	2.40	0.54
1:A:291:LEU:C	1:A:291:LEU:HD12	2.28	0.54
1:D:83:GLU:OE1	1:D:100:HIS:ND1	2.41	0.54
1:E:69:VAL:CG2	1:E:118:VAL:HG22	2.38	0.54
1:I:77:ILE:O	1:I:81:VAL:HG23	2.06	0.54
1:I:714:LEU:HD12	1:I:717:LEU:HD12	1.89	0.54
1:K:120:GLU:O	1:K:124:THR:HG23	2.07	0.54
1:L:294:ARG:NH2	1:L:479:ASP:OD2	2.40	0.54
1:H:23:LEU:HD22	1:H:88:LYS:HE3	1.89	0.54
1:H:266:ASP:OD2	1:H:268:TRP:NE1	2.38	0.54
1:J:639:LEU:HD23	1:J:639:LEU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:HIS:HB2	1:K:55:GLU:CD	2.27	0.54
1:A:224:PHE:O	1:A:228:ILE:HG22	2.08	0.54
1:B:136:ASP:OD1	1:B:137:LEU:N	2.38	0.54
1:B:174:ASN:ND2	1:B:284:ASN:O	2.39	0.54
1:B:701:ASP:OD1	1:B:702:ASN:N	2.40	0.54
1:D:450:ASP:C	1:D:450:ASP:OD1	2.45	0.54
1:E:686:ASN:O	1:E:686:ASN:OD1	2.25	0.54
1:E:753:THR:HB	1:E:755:LEU:HG	1.90	0.54
1:F:841:GLN:NE2	1:F:874:ILE:CB	2.71	0.54
1:H:828:LYS:O	1:H:851:THR:OG1	2.16	0.54
1:I:767:GLU:OE1	1:I:767:GLU:N	2.38	0.54
1:A:469:ASP:OD1	1:A:469:ASP:N	2.40	0.54
1:B:34:LEU:HD23	1:B:118:VAL:HG21	1.89	0.54
1:E:254:LEU:HD22	1:E:281:PRO:CD	2.37	0.54
1:H:399:ASP:C	1:H:399:ASP:OD1	2.45	0.54
1:L:166:ILE:HG23	1:L:202:ILE:HD11	1.89	0.54
1:L:876:PHE:O	1:L:877:LYS:NZ	2.39	0.54
1:A:74:GLU:O	1:A:78:ASP:OD2	2.26	0.54
1:A:803:LEU:HD23	1:A:827:LEU:HD13	1.89	0.54
1:B:476:ARG:NH2	1:B:479:ASP:OD1	2.40	0.54
1:C:782:GLU:O	1:C:804:VAL:N	2.36	0.54
1:D:6:VAL:HG21	1:D:45:LEU:HD11	1.89	0.54
1:G:119:ARG:HA	1:G:122:ARG:HG3	1.89	0.54
1:G:169:LEU:HD11	1:G:206:PHE:CE2	2.42	0.54
1:H:30:ALA:O	1:H:34:LEU:HG	2.07	0.54
1:J:82:ILE:O	1:J:86:LEU:HD23	2.07	0.54
1:K:56:ASN:HB3	1:K:59:LEU:HD22	1.90	0.54
1:K:154:ASP:OD1	1:K:154:ASP:C	2.45	0.54
1:L:105:LYS:O	1:L:108:ALA:HB3	2.08	0.54
1:C:6:VAL:HG22	1:C:70:VAL:HG21	1.88	0.54
1:C:136:ASP:OD1	1:C:137:LEU:N	2.40	0.54
1:G:103:ARG:O	1:G:107:VAL:HG23	2.07	0.54
1:J:732:LYS:NZ	1:J:780:SER:OG	2.39	0.54
1:L:170:LEU:HD11	1:L:205:GLU:OE2	2.06	0.54
1:B:637:ARG:O	1:B:638:HIS:ND1	2.40	0.54
1:D:262:VAL:HG23	1:D:289:VAL:HG22	1.89	0.54
1:F:651:VAL:O	1:F:651:VAL:HG13	2.08	0.54
1:I:225:LEU:O	1:I:225:LEU:HD23	2.07	0.54
1:J:205:GLU:OE2	1:J:259:LYS:NZ	2.29	0.54
1:K:103:ARG:HD3	1:K:103:ARG:C	2.28	0.54
1:B:735:LEU:CD1	1:B:763:LEU:HD21	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:845:LEU:HD11	1:C:856:ALA:CB	2.38	0.54
1:D:80:PHE:HB2	1:D:111:ILE:HD11	1.89	0.54
1:G:309:LEU:HD12	1:G:310:LYS:H	1.72	0.54
1:F:841:GLN:CG	1:F:875:ALA:O	2.53	0.54
1:I:173:SER:HA	1:I:286:PRO:HB3	1.89	0.54
1:J:21:VAL:O	1:J:25:SER:N	2.40	0.54
1:J:102:LYS:HA	1:J:106:GLU:HB3	1.88	0.54
1:J:172:GLU:O	1:J:288:ARG:NH2	2.41	0.54
1:J:178:VAL:HG21	1:J:302:CYS:HB3	1.89	0.54
1:L:449:GLU:OE2	1:L:449:GLU:O	2.24	0.54
1:C:828:LYS:O	1:C:851:THR:HG23	2.08	0.54
1:D:591:TYR:CE1	1:D:614:THR:HG21	2.43	0.54
1:E:732:LYS:NZ	1:E:780:SER:OG	2.41	0.54
1:F:829:GLU:OE1	1:F:830:VAL:N	2.41	0.54
1:G:233:ARG:CZ	1:G:233:ARG:HA	2.37	0.54
1:H:173:SER:HA	1:H:286:PRO:HB3	1.90	0.54
1:I:483:GLU:OE1	1:I:484:PHE:N	2.41	0.54
1:L:501:LEU:HA	1:L:505:GLN:OE1	2.09	0.54
1:A:18:ARG:NH1	1:E:739:TYR:O	2.42	0.53
1:A:65:LYS:O	1:A:69:VAL:HG23	2.08	0.53
1:B:725:ASP:OD1	1:B:726:SER:N	2.41	0.53
1:D:504:GLU:OE1	1:D:505:GLN:NE2	2.41	0.53
1:J:80:PHE:HB2	1:J:111:ILE:HD11	1.89	0.53
1:J:102:LYS:CB	1:J:106:GLU:HB3	2.38	0.53
1:K:92:VAL:HG12	1:K:94:ARG:H	1.73	0.53
1:B:95:VAL:O	1:B:96:LEU:HD23	2.07	0.53
1:F:262:VAL:HG23	1:F:289:VAL:HG22	1.90	0.53
1:F:580:SER:HG	1:F:583:PHE:HD1	1.56	0.53
1:I:469:ASP:OD1	1:I:469:ASP:N	2.41	0.53
1:K:174:ASN:ND2	1:K:284:ASN:OD1	2.36	0.53
1:K:590:ARG:HA	1:K:612:ILE:HA	1.90	0.53
1:K:755:LEU:O	1:K:780:SER:N	2.40	0.53
1:L:83:GLU:CG	1:L:104:VAL:HG22	2.38	0.53
1:A:610:TRP:CH2	1:A:611:ASN:OD1	2.61	0.53
1:A:714:LEU:CD1	1:A:717:LEU:HD12	2.39	0.53
1:E:645:ALA:O	1:E:672:ALA:N	2.40	0.53
1:E:681:PHE:CE1	1:E:714:LEU:HD11	2.43	0.53
1:E:687:LEU:HD23	1:E:688:LYS:N	2.23	0.53
1:F:857:ARG:O	1:F:857:ARG:HD3	2.08	0.53
1:G:73:ALA:HB2	1:G:114:ILE:HG21	1.89	0.53
1:H:325:VAL:HG23	1:H:361:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:ARG:NH1	1:J:739:TYR:O	2.41	0.53
1:A:325:VAL:HG23	1:A:361:ILE:HG23	1.90	0.53
1:A:350:PRO:O	1:A:354:VAL:HG23	2.07	0.53
1:B:33:SER:O	1:B:37:ASP:OD1	2.26	0.53
1:D:295:ASP:OD1	1:D:296:SER:N	2.41	0.53
1:E:705:ALA:O	1:E:707:SER:N	2.41	0.53
1:F:841:GLN:CD	1:F:874:ILE:HG21	2.29	0.53
1:K:52:HIS:HB2	1:K:55:GLU:HG3	1.90	0.53
1:B:208:THR:OG1	1:B:259:LYS:O	2.26	0.53
1:C:381:LEU:HD23	1:C:393:LEU:HD21	1.91	0.53
1:E:647:LEU:HD11	1:E:668:LEU:HD13	1.90	0.53
1:H:291:LEU:C	1:H:291:LEU:HD12	2.29	0.53
1:K:74:GLU:O	1:K:78:ASP:OD2	2.27	0.53
1:L:83:GLU:HG2	1:L:104:VAL:HG22	1.90	0.53
1:A:797:TRP:CD2	1:A:820:VAL:HG11	2.44	0.53
1:C:445:GLU:OE1	1:C:445:GLU:N	2.38	0.53
1:D:88:LYS:HD2	1:D:88:LYS:N	2.23	0.53
1:D:192:LEU:HD11	1:D:196:ILE:HD11	1.91	0.53
1:D:505:GLN:OE1	1:D:505:GLN:N	2.42	0.53
1:E:117:LYS:O	1:E:120:GLU:O	2.27	0.53
1:G:846:GLN:HB2	1:G:881:PHE:HD2	1.69	0.53
1:I:73:ALA:HA	1:I:114:ILE:HG21	1.90	0.53
1:J:254:LEU:HD12	1:J:260:TYR:CG	2.44	0.53
1:K:57:GLU:HA	1:K:60:ARG:NH1	2.24	0.53
1:E:334:GLU:OE1	1:E:334:GLU:N	2.33	0.53
1:H:259:LYS:NZ	1:H:286:PRO:O	2.41	0.53
1:I:700:LEU:HB2	1:I:733:LEU:HD22	1.91	0.53
1:A:66:ILE:HD13	1:A:121:ILE:HG21	1.91	0.53
1:B:446:CYS:O	1:B:450:ASP:OD2	2.27	0.53
1:E:860:GLN:OE1	1:E:861:ALA:N	2.42	0.53
1:F:169:LEU:HD12	1:F:206:PHE:CE2	2.43	0.53
1:F:259:LYS:HD3	1:F:285:LYS:HD3	1.90	0.53
1:F:678:GLU:OE1	1:F:678:GLU:N	2.37	0.53
1:G:158:PHE:CE1	1:G:309:LEU:HD11	2.43	0.53
1:G:235:THR:O	1:G:235:THR:HG22	2.08	0.53
1:J:80:PHE:CD2	1:J:106:GLU:HG2	2.43	0.53
1:K:103:ARG:NH1	1:K:107:VAL:HG12	2.24	0.53
1:L:192:LEU:HD11	1:L:196:ILE:HD11	1.90	0.53
1:H:62:LEU:HD12	1:H:65:LYS:HD3	1.90	0.53
1:J:24:ILE:HG22	1:J:28:LYS:HA	1.90	0.53
1:B:662:ASN:OD1	1:B:665:LEU:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ILE:HD11	1:B:690:LEU:HD11	1.90	0.53
1:C:83:GLU:CG	1:C:104:VAL:HG22	2.38	0.53
1:H:9:LEU:HD23	1:H:38:LEU:HD21	1.91	0.53
1:I:701:ASP:OD1	1:I:703:LYS:N	2.37	0.53
1:I:752:ASP:N	1:I:776:GLU:OE1	2.42	0.53
1:J:735:LEU:HD13	1:J:763:LEU:HD21	1.91	0.53
1:K:416:PRO:CG	1:K:544:PHE:HB2	2.39	0.53
1:B:409:PHE:HE1	1:B:477:LEU:HD21	1.74	0.52
1:D:413:SER:CB	1:D:485:CYS:HB2	2.39	0.52
1:F:544:PHE:CE1	1:F:570:ASP:OD2	2.62	0.52
1:F:843:MET:CE	1:F:856:ALA:HB1	2.39	0.52
1:I:692:ILE:HD13	1:I:699:LEU:HD11	1.91	0.52
1:I:828:LYS:O	1:I:851:THR:OG1	2.14	0.52
1:C:169:LEU:O	1:C:170:LEU:HB2	2.09	0.52
1:D:101:TYR:O	1:D:104:VAL:HG22	2.09	0.52
1:E:208:THR:OG1	1:E:259:LYS:O	2.27	0.52
1:F:87:HIS:CD2	1:F:104:VAL:HG21	2.44	0.52
1:I:219:ARG:HD2	1:I:222:GLU:CD	2.29	0.52
1:J:696:ILE:HD11	1:J:723:ILE:O	2.09	0.52
1:K:644:SER:O	1:K:644:SER:OG	2.27	0.52
1:L:211:TRP:CZ3	1:L:263:VAL:HG11	2.44	0.52
1:A:255:GLY:O	1:A:285:LYS:NZ	2.42	0.52
1:G:169:LEU:O	1:G:170:LEU:HB2	2.08	0.52
1:G:233:ARG:HA	1:G:233:ARG:NE	2.25	0.52
1:G:295:ASP:OD1	1:G:296:SER:N	2.43	0.52
1:H:172:GLU:HG3	1:H:172:GLU:O	2.09	0.52
1:I:539:ARG:O	1:I:566:LEU:HD23	2.09	0.52
1:J:192:LEU:HD11	1:J:196:ILE:HD11	1.92	0.52
1:B:29:GLU:OE1	1:B:29:GLU:N	2.38	0.52
1:E:478:HIS:HB3	1:E:481:LEU:HD23	1.92	0.52
1:I:681:PHE:CD1	1:I:714:LEU:HD11	2.44	0.52
1:K:166:ILE:HG12	1:K:202:ILE:HD11	1.90	0.52
1:A:6:VAL:O	1:A:10:VAL:HG23	2.10	0.52
1:B:16:LEU:HD23	1:B:24:ILE:HD11	1.92	0.52
1:B:63:VAL:HA	1:B:66:ILE:HD12	1.91	0.52
1:C:27:VAL:HG11	1:C:111:ILE:HD12	1.91	0.52
1:C:45:LEU:CD2	1:C:63:VAL:HG13	2.38	0.52
1:D:45:LEU:HD22	1:D:63:VAL:HG13	1.91	0.52
1:G:700:LEU:HD21	1:G:735:LEU:HD23	1.91	0.52
1:H:677:THR:HG22	1:H:678:GLU:H	1.75	0.52
1:I:178:VAL:HG13	1:I:289:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:ASP:O	1:K:137:LEU:HD22	2.09	0.52
1:L:401:LEU:HD23	1:L:406:LYS:HA	1.91	0.52
1:B:753:THR:OG1	1:B:778:GLY:O	2.28	0.52
1:C:341:SER:OG	1:C:374:ASP:OD2	2.25	0.52
1:D:88:LYS:HD2	1:D:88:LYS:H	1.74	0.52
1:D:756:GLU:OE1	1:D:756:GLU:N	2.39	0.52
1:G:64:LYS:HD3	1:G:65:LYS:H	1.74	0.52
1:G:414:ALA:HB2	1:G:496:PHE:CE2	2.44	0.52
1:I:241:MET:HG3	1:I:245:ASP:HB2	1.91	0.52
1:I:721:LYS:HG2	1:I:749:THR:HB	1.92	0.52
1:F:526:LEU:HD11	1:F:552:PRO:CD	2.39	0.52
1:H:735:LEU:CD1	1:H:763:LEU:HD21	2.40	0.52
1:C:821:LEU:HD21	1:C:827:LEU:CD2	2.40	0.52
1:D:252:GLU:OE2	1:D:256:LYS:HE3	2.09	0.52
1:E:416:PRO:HD3	1:E:544:PHE:HD2	1.74	0.52
1:E:756:GLU:HB2	1:E:758:LYS:HG2	1.92	0.52
1:E:823:CYS:N	1:E:846:GLN:OE1	2.43	0.52
1:F:117:LYS:O	1:F:121:ILE:HG12	2.10	0.52
1:F:810:ALA:N	1:F:833:ALA:HB1	2.25	0.52
1:G:211:TRP:CZ3	1:G:263:VAL:HG11	2.45	0.52
1:L:80:PHE:CE2	1:L:108:ALA:HB2	2.44	0.52
1:A:219:ARG:HD2	1:A:222:GLU:CD	2.31	0.52
1:A:756:GLU:OE1	1:A:756:GLU:N	2.40	0.52
1:C:660:LEU:HD23	1:C:660:LEU:H	1.73	0.52
1:J:16:LEU:HD23	1:J:24:ILE:HD11	1.92	0.52
1:J:241:MET:HE3	1:J:245:ASP:HB3	1.91	0.52
1:K:771:VAL:HG22	1:K:795:VAL:HG12	1.92	0.52
1:L:295:ASP:OD1	1:L:296:SER:N	2.43	0.52
1:L:750:LEU:HD23	1:L:753:THR:HG21	1.91	0.52
1:B:350:PRO:HB3	3:B:902:ADP:N3	2.25	0.52
1:C:704:SER:O	1:C:705:ALA:HB3	2.10	0.52
1:F:505:GLN:OE1	1:F:505:GLN:N	2.41	0.52
1:H:701:ASP:OD1	1:H:703:LYS:N	2.40	0.52
1:J:238:TYR:HH	1:J:253:PHE:HE2	1.58	0.52
1:C:178:VAL:CG1	1:C:303:ASN:HB2	2.40	0.51
1:D:630:ILE:HD11	1:D:647:LEU:CD1	2.39	0.51
1:E:609:LEU:HD12	1:E:609:LEU:H	1.75	0.51
1:F:345:LYS:HD3	1:F:377:VAL:HG13	1.91	0.51
1:G:111:ILE:HA	1:G:114:ILE:HD12	1.92	0.51
1:G:755:LEU:O	1:G:780:SER:N	2.38	0.51
1:H:148:PRO:HG3	1:H:453:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:735:LEU:HD13	1:H:763:LEU:HD21	1.92	0.51
1:I:6:VAL:O	1:I:10:VAL:HG23	2.10	0.51
1:I:82:ILE:CD1	1:I:565:LEU:CD2	2.88	0.51
1:K:64:LYS:HG3	1:K:65:LYS:HG3	1.92	0.51
1:A:755:LEU:HD12	1:A:779:PHE:HE1	1.75	0.51
1:A:837:ILE:O	1:A:863:LYS:NZ	2.42	0.51
1:B:21:VAL:O	1:B:25:SER:N	2.43	0.51
1:D:409:PHE:O	1:D:485:CYS:HB3	2.10	0.51
1:D:755:LEU:O	1:D:780:SER:N	2.41	0.51
1:F:526:LEU:HD23	1:F:549:ILE:HG21	1.92	0.51
1:K:170:LEU:HD21	1:K:206:PHE:CZ	2.46	0.51
1:B:341:SER:O	1:B:345:LYS:HG3	2.10	0.51
1:C:58:VAL:O	1:C:62:LEU:HG	2.10	0.51
1:F:192:LEU:HD11	1:F:196:ILE:HD11	1.92	0.51
1:F:858:GLN:OE1	1:F:858:GLN:HA	2.11	0.51
1:H:115:ARG:NH1	1:H:119:ARG:HB2	2.25	0.51
1:H:255:GLY:O	1:H:285:LYS:NZ	2.43	0.51
1:J:670:THR:HG21	1:J:693:ARG:HE	1.74	0.51
1:L:176:LEU:HD11	1:L:260:TYR:OH	2.11	0.51
1:A:178:VAL:HG21	1:A:302:CYS:HB3	1.92	0.51
1:A:653:PRO:HD3	1:A:660:LEU:HD11	1.92	0.51
1:F:103:ARG:HD3	1:F:103:ARG:C	2.31	0.51
1:G:816:LEU:HD23	1:G:817:LYS:N	2.26	0.51
1:H:175:HIS:O	1:H:288:ARG:NH1	2.42	0.51
1:H:467:THR:HG23	2:H:901:IHP:P5	2.51	0.51
1:J:108:ALA:O	1:J:112:LYS:HG2	2.10	0.51
1:C:119:ARG:HA	1:C:122:ARG:HG3	1.93	0.51
1:C:595:SER:O	1:C:596:SER:OG	2.28	0.51
1:I:415:PHE:CE2	1:I:544:PHE:CZ	2.98	0.51
1:I:735:LEU:HD13	1:I:763:LEU:HD21	1.92	0.51
1:K:766:LEU:HD13	1:K:769:LEU:HD12	1.92	0.51
1:A:225:LEU:CD2	1:A:246:LEU:CD1	2.89	0.51
1:A:844:MET:SD	1:A:881:PHE:CE2	3.04	0.51
1:B:172:GLU:OE2	1:B:175:HIS:HB3	2.10	0.51
1:D:350:PRO:HB3	3:D:902:ADP:C4	2.45	0.51
1:E:105:LYS:HA	1:E:108:ALA:HB3	1.93	0.51
1:J:612:ILE:HD12	1:J:615:ILE:HD11	1.93	0.51
1:L:149:VAL:HG12	1:L:150:VAL:N	2.25	0.51
1:L:184:MET:O	1:L:189:LYS:NZ	2.24	0.51
1:A:37:ASP:OD2	1:A:122:ARG:NH1	2.44	0.51
1:A:701:ASP:O	1:A:705:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:THR:HG23	1:C:689:LYS:HG2	1.91	0.51
1:E:630:ILE:HA	1:E:633:MET:CE	2.41	0.51
1:F:705:ALA:O	1:F:707:SER:N	2.43	0.51
1:H:717:LEU:HD23	1:H:718:GLU:N	2.26	0.51
1:I:92:VAL:HG11	1:I:97:ASP:CB	2.40	0.51
1:L:108:ALA:HA	1:L:111:ILE:HG12	1.92	0.51
1:L:463:VAL:HG13	1:L:472:ILE:HG23	1.91	0.51
1:B:149:VAL:HG12	1:B:150:VAL:N	2.25	0.51
1:B:315:ASP:OD1	1:B:316:GLU:N	2.43	0.51
1:B:645:ALA:O	1:B:672:ALA:N	2.44	0.51
1:H:800:ARG:NH1	1:H:823:CYS:SG	2.84	0.51
1:J:273:TRP:HA	1:J:276:ILE:HG22	1.92	0.51
1:L:37:ASP:OD2	1:L:115:ARG:NH2	2.44	0.51
1:B:453:ASN:O	1:B:457:ASN:OD1	2.29	0.51
1:C:202:ILE:HG22	1:C:209:ARG:HD2	1.92	0.51
1:H:795:VAL:HG22	1:H:818:HIS:HB3	1.92	0.51
1:I:413:SER:HB3	1:I:485:CYS:HB3	1.93	0.51
1:K:136:ASP:C	1:K:137:LEU:HD22	2.32	0.51
1:A:244:GLU:OE2	1:A:244:GLU:HA	2.11	0.51
1:A:735:LEU:CD1	1:A:763:LEU:HD21	2.40	0.51
1:B:816:LEU:HD23	1:B:817:LYS:N	2.25	0.51
1:E:403:TYR:HA	1:E:406:LYS:HB2	1.93	0.51
1:F:369:GLU:O	1:F:373:VAL:HG23	2.11	0.51
1:I:64:LYS:O	1:I:65:LYS:HG2	2.11	0.51
1:I:176:LEU:HD23	1:I:277:LYS:NZ	2.26	0.51
1:I:641:THR:OG1	1:I:642:ASN:N	2.44	0.51
1:L:34:LEU:HD12	1:L:118:VAL:HG11	1.92	0.51
1:B:169:LEU:HD11	1:B:170:LEU:CD1	2.40	0.50
1:E:172:GLU:O	1:E:288:ARG:NH2	2.44	0.50
1:F:390:CYS:O	1:F:394:VAL:HG23	2.11	0.50
1:A:173:SER:HA	1:A:286:PRO:HB3	1.94	0.50
1:C:176:LEU:HD11	1:C:260:TYR:HH	1.75	0.50
1:C:633:MET:HE3	1:C:636:LEU:HD22	1.93	0.50
1:D:45:LEU:CD2	1:D:63:VAL:HG13	2.41	0.50
1:E:176:LEU:HD13	1:E:260:TYR:OH	2.12	0.50
1:E:741:PHE:CD2	1:E:766:LEU:HD11	2.43	0.50
1:H:90:LYS:HB3	1:H:92:VAL:HG23	1.93	0.50
1:H:412:CYS:SG	1:H:477:LEU:HD21	2.51	0.50
1:K:499:ILE:O	1:K:499:ILE:HG13	2.12	0.50
1:K:750:LEU:HD22	1:K:753:THR:OG1	2.11	0.50
1:L:665:LEU:HD23	1:L:666:GLN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD21	1:A:246:LEU:HD11	1.92	0.50
1:A:816:LEU:O	1:A:839:SER:OG	2.16	0.50
1:B:333:PRO:HA	1:B:336:VAL:HG23	1.94	0.50
1:B:735:LEU:HD13	1:B:763:LEU:HD21	1.93	0.50
1:C:76:ALA:HB1	1:C:111:ILE:HG23	1.93	0.50
1:C:555:ASP:OD1	1:C:558:THR:HG21	2.11	0.50
1:E:172:GLU:O	1:E:172:GLU:HG3	2.10	0.50
1:E:433:GLU:CD	1:E:568:VAL:HG21	2.31	0.50
1:G:174:ASN:ND2	1:G:284:ASN:HB3	2.25	0.50
1:I:345:LYS:O	1:I:381:LEU:HD23	2.10	0.50
1:I:501:LEU:HD11	1:I:507:PHE:CD1	2.46	0.50
1:K:92:VAL:HG11	1:K:98:LEU:H	1.76	0.50
1:B:596:SER:OG	1:B:597:ASP:N	2.45	0.50
1:B:718:GLU:O	1:B:718:GLU:CG	2.59	0.50
1:E:595:SER:OG	1:E:596:SER:N	2.44	0.50
1:G:174:ASN:HA	1:G:284:ASN:C	2.32	0.50
1:K:64:LYS:HZ2	1:K:64:LYS:HA	1.77	0.50
1:E:27:VAL:HG23	1:E:27:VAL:O	2.11	0.50
1:E:639:LEU:HD23	1:E:639:LEU:O	2.12	0.50
1:F:53:ILE:HA	1:F:59:LEU:HD21	1.94	0.50
1:J:642:ASN:OD1	1:J:643:SER:N	2.44	0.50
1:K:145:ARG:NH2	1:K:361:ILE:HG12	2.26	0.50
1:L:725:ASP:OD1	1:L:726:SER:N	2.45	0.50
1:B:149:VAL:CG1	1:B:150:VAL:N	2.75	0.50
1:B:695:LYS:HD2	1:B:698:VAL:HG23	1.93	0.50
1:G:176:LEU:HD11	1:G:260:TYR:OH	2.12	0.50
1:G:401:LEU:O	1:G:406:LYS:HE3	2.12	0.50
1:H:56:ASN:O	1:H:60:ARG:HG3	2.11	0.50
1:H:148:PRO:HB3	1:H:457:ASN:OD1	2.11	0.50
1:H:413:SER:HB3	1:H:485:CYS:HB3	1.94	0.50
1:I:176:LEU:HD13	1:I:287:ASN:CG	2.32	0.50
1:A:844:MET:CE	1:A:881:PHE:HE2	2.25	0.50
1:B:321:LEU:O	1:B:325:VAL:HG23	2.11	0.50
1:E:416:PRO:HD3	1:E:544:PHE:CD2	2.47	0.50
1:F:129:LEU:HD12	1:F:129:LEU:O	2.11	0.50
1:G:34:LEU:O	1:G:38:LEU:HG	2.12	0.50
1:H:797:TRP:CD2	1:H:820:VAL:HG11	2.47	0.50
1:I:523:SER:OG	1:I:524:SER:N	2.44	0.50
1:I:665:LEU:HD23	1:I:666:GLN:N	2.27	0.50
1:I:756:GLU:OE1	1:I:756:GLU:N	2.42	0.50
1:I:797:TRP:CD2	1:I:820:VAL:HG11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:OE1	1:A:29:GLU:N	2.35	0.50
1:A:445:GLU:OE1	1:A:445:GLU:N	2.44	0.50
1:C:40:ASP:OD2	1:C:122:ARG:NH2	2.45	0.50
1:C:174:ASN:HA	1:C:284:ASN:O	2.11	0.50
1:C:721:LYS:NZ	1:C:749:THR:HG21	2.27	0.50
1:F:221:ARG:NH2	1:F:239:HIS:O	2.44	0.50
1:G:11:GLU:C	1:G:11:GLU:OE2	2.50	0.50
1:H:154:ASP:OD2	1:H:323:LYS:NZ	2.44	0.50
1:I:244:GLU:OE2	1:I:244:GLU:HA	2.12	0.50
1:J:645:ALA:O	1:J:672:ALA:N	2.44	0.50
1:K:369:GLU:O	1:K:373:VAL:HG23	2.11	0.50
1:K:795:VAL:HG23	1:K:818:HIS:HB3	1.93	0.50
1:L:354:VAL:HG21	3:L:902:ADP:H8	1.76	0.50
1:L:845:LEU:HB3	1:L:880:ILE:HG23	1.92	0.50
1:A:201:LYS:O	1:A:205:GLU:OE1	2.30	0.50
1:A:401:LEU:HD12	1:A:458:ARG:HH12	1.76	0.50
1:C:152:GLU:HG2	1:C:323:LYS:HB3	1.94	0.50
1:C:161:GLU:OE1	1:C:307:HIS:NE2	2.44	0.50
1:C:178:VAL:HG11	1:C:302:CYS:HB3	1.93	0.50
1:C:599:ILE:HG23	1:C:599:ILE:O	2.12	0.50
1:C:612:ILE:HD12	1:C:615:ILE:HD11	1.94	0.50
1:F:177:GLU:HG2	1:F:288:ARG:NH1	2.27	0.50
1:F:402:PRO:HG2	1:F:405:LEU:HD23	1.93	0.50
1:I:835:ALA:O	1:I:866:GLN:NE2	2.37	0.50
1:L:155:VAL:HG13	3:L:902:ADP:HN62	1.75	0.50
1:L:408:CYS:O	1:L:412:CYS:HB2	2.11	0.50
1:A:155:VAL:HG12	3:A:902:ADP:N6	2.27	0.49
1:B:244:GLU:OE1	1:B:245:ASP:N	2.45	0.49
1:F:609:LEU:H	1:F:609:LEU:HD12	1.77	0.49
1:H:345:LYS:NZ	1:H:374:ASP:OD1	2.45	0.49
1:I:10:VAL:HG22	1:I:38:LEU:HB3	1.92	0.49
1:I:647:LEU:CD1	1:I:671:ILE:HD12	2.42	0.49
1:J:321:LEU:O	1:J:325:VAL:HG23	2.12	0.49
1:A:56:ASN:OD1	1:A:58:VAL:N	2.44	0.49
1:A:539:ARG:O	1:A:566:LEU:HD23	2.12	0.49
1:C:188:GLY:HA3	3:C:902:ADP:C8	2.47	0.49
1:C:393:LEU:HD23	1:C:396:MET:CE	2.41	0.49
1:F:8:PHE:CE1	1:F:12:ASN:OD1	2.65	0.49
1:G:37:ASP:O	1:G:40:ASP:OD1	2.29	0.49
1:G:670:THR:HG21	1:G:693:ARG:HE	1.76	0.49
1:I:92:VAL:HG11	1:I:97:ASP:CG	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:ALA:O	1:I:117:LYS:HG3	2.12	0.49
1:J:531:THR:HG22	1:J:531:THR:O	2.11	0.49
1:L:531:THR:HG22	1:L:531:THR:O	2.12	0.49
1:A:161:GLU:OE1	1:A:307:HIS:NE2	2.45	0.49
1:B:83:GLU:HB3	1:B:104:VAL:HG22	1.95	0.49
1:B:119:ARG:CZ	1:B:123:GLN:HE22	2.25	0.49
1:C:641:THR:HG23	1:C:670:THR:HB	1.93	0.49
1:D:725:ASP:OD1	1:D:726:SER:N	2.45	0.49
1:E:33:SER:O	1:E:37:ASP:OD1	2.29	0.49
1:E:599:ILE:HG23	1:E:599:ILE:O	2.12	0.49
1:F:755:LEU:O	1:F:780:SER:N	2.41	0.49
1:H:244:GLU:HA	1:H:244:GLU:OE2	2.12	0.49
1:I:402:PRO:HD2	1:I:405:LEU:HD12	1.95	0.49
1:I:800:ARG:NE	1:I:800:ARG:HA	2.27	0.49
1:L:95:VAL:O	1:L:96:LEU:HD23	2.12	0.49
1:A:350:PRO:HB2	3:A:902:ADP:C8	2.47	0.49
1:A:856:ALA:HA	1:A:859:ILE:HD12	1.93	0.49
1:C:6:VAL:HG21	1:C:45:LEU:CD1	2.43	0.49
1:D:41:PHE:CZ	1:D:122:ARG:HG3	2.47	0.49
1:E:718:GLU:CG	1:E:718:GLU:O	2.60	0.49
1:F:115:ARG:O	1:F:118:VAL:HG22	2.11	0.49
1:F:350:PRO:HB2	3:F:902:ADP:C8	2.48	0.49
1:I:544:PHE:CE1	1:I:570:ASP:OD2	2.66	0.49
1:A:715:GLU:O	1:A:744:LYS:NZ	2.36	0.49
1:B:219:ARG:HB2	1:B:222:GLU:OE1	2.13	0.49
1:C:59:LEU:HD22	1:C:132:LEU:HD21	1.94	0.49
1:D:172:GLU:HG3	1:D:172:GLU:O	2.11	0.49
1:E:80:PHE:HB2	1:E:111:ILE:HD11	1.93	0.49
1:F:24:ILE:HG22	1:F:24:ILE:O	2.11	0.49
1:F:426:LEU:HG	1:F:430:TRP:CZ2	2.48	0.49
1:F:698:VAL:O	1:F:704:SER:OG	2.25	0.49
1:I:92:VAL:HG11	1:I:97:ASP:HB2	1.95	0.49
1:K:169:LEU:HD12	1:K:169:LEU:O	2.13	0.49
1:K:777:ASN:N	1:K:800:ARG:O	2.45	0.49
1:A:208:THR:OG1	1:A:259:LYS:O	2.30	0.49
1:C:52:HIS:O	1:C:59:LEU:HD12	2.13	0.49
1:C:405:LEU:HD12	1:C:455:LEU:HD21	1.94	0.49
1:F:136:ASP:C	1:F:137:LEU:HD12	2.33	0.49
1:F:172:GLU:O	1:F:288:ARG:NH2	2.45	0.49
1:H:169:LEU:C	1:H:170:LEU:HG	2.32	0.49
1:I:735:LEU:CD1	1:I:763:LEU:HD21	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:34:LEU:HD23	1:J:118:VAL:HG21	1.94	0.49
1:J:173:SER:HA	1:J:286:PRO:HB3	1.93	0.49
1:K:145:ARG:NH1	1:K:457:ASN:HB2	2.28	0.49
1:D:467:THR:OG1	1:D:471:GLN:N	2.46	0.49
1:D:866:GLN:O	1:D:871:THR:OG1	2.30	0.49
1:H:80:PHE:HD2	1:H:111:ILE:HD13	1.77	0.49
1:I:117:LYS:O	1:I:121:ILE:HG12	2.12	0.49
1:K:169:LEU:O	1:K:170:LEU:HB2	2.12	0.49
1:K:862:LYS:O	1:K:866:GLN:HG3	2.11	0.49
1:L:9:LEU:HD23	1:L:70:VAL:HG23	1.94	0.49
1:L:64:LYS:HD3	1:L:65:LYS:H	1.78	0.49
1:B:607:GLY:HA2	1:B:633:MET:CE	2.43	0.49
1:B:728:ILE:O	1:B:728:ILE:CG1	2.60	0.49
1:D:211:TRP:CZ3	1:D:263:VAL:HG11	2.48	0.49
1:D:255:GLY:O	1:D:285:LYS:NZ	2.45	0.49
1:E:82:ILE:O	1:E:86:LEU:HD23	2.13	0.49
1:K:592:VAL:HG13	1:K:592:VAL:O	2.12	0.49
1:L:129:LEU:HD23	1:L:129:LEU:H	1.78	0.49
1:L:172:GLU:HG3	1:L:172:GLU:O	2.13	0.49
1:A:120:GLU:OE1	1:A:121:ILE:N	2.46	0.49
1:A:660:LEU:HD13	1:A:683:ARG:NH2	2.28	0.49
1:B:15:GLN:O	1:B:19:ASP:OD2	2.31	0.49
1:F:21:VAL:O	1:F:25:SER:N	2.46	0.49
1:F:821:LEU:HD12	1:F:845:LEU:CD2	2.43	0.49
1:F:841:GLN:NE2	1:F:874:ILE:HD12	2.28	0.49
1:G:483:GLU:OE1	1:G:484:PHE:N	2.46	0.49
1:G:725:ASP:OD1	1:G:726:SER:N	2.46	0.49
1:H:360:LEU:HD11	1:H:373:VAL:HG21	1.94	0.49
1:H:788:GLY:N	1:H:812:ASP:OD1	2.46	0.49
1:K:179:VAL:HG23	1:K:179:VAL:O	2.11	0.49
1:K:330:LYS:HA	1:K:330:LYS:HE3	1.95	0.49
1:K:390:CYS:O	1:K:394:VAL:HG23	2.12	0.49
1:A:643:SER:OG	1:A:644:SER:N	2.45	0.49
1:C:820:VAL:HG13	1:C:822:ILE:HD11	1.91	0.49
1:E:416:PRO:HG3	1:E:522:HIS:CD2	2.48	0.49
1:F:113:ALA:HB1	1:F:117:LYS:NZ	2.28	0.49
1:G:113:ALA:O	1:G:117:LYS:HG3	2.13	0.49
1:G:881:PHE:HB2	1:G:882:PRO:HD3	1.95	0.49
1:I:74:GLU:O	1:I:78:ASP:OD2	2.31	0.49
1:J:221:ARG:NH2	1:J:239:HIS:O	2.45	0.49
1:K:544:PHE:CE1	1:K:570:ASP:OD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:788:GLY:N	1:K:812:ASP:OD1	2.46	0.49
1:C:380:HIS:CB	1:C:396:MET:HE1	2.41	0.48
1:E:82:ILE:CD1	1:E:565:LEU:HD22	2.43	0.48
1:E:429:LEU:HD23	1:E:591:TYR:CD2	2.48	0.48
1:E:469:ASP:N	1:E:469:ASP:OD1	2.46	0.48
1:F:429:LEU:O	1:F:433:GLU:HG2	2.13	0.48
1:H:92:VAL:HG21	1:H:97:ASP:CG	2.33	0.48
1:I:642:ASN:O	1:I:693:ARG:NE	2.46	0.48
1:I:838:ARG:CZ	1:I:838:ARG:HA	2.42	0.48
1:J:47:GLN:HB3	1:J:132:LEU:HD13	1.95	0.48
1:K:794:LEU:HD23	1:K:817:LYS:HD2	1.95	0.48
1:A:795:VAL:HG22	1:A:818:HIS:HB3	1.95	0.48
1:D:155:VAL:HG12	3:D:902:ADP:N6	2.27	0.48
1:D:773:LYS:HG2	1:D:797:TRP:HB3	1.95	0.48
1:F:841:GLN:NE2	1:F:874:ILE:HB	2.28	0.48
1:I:110:GLU:O	1:I:114:ILE:HG12	2.13	0.48
1:A:425:LYS:CE	1:A:572:GLU:OE2	2.61	0.48
1:B:173:SER:HB2	1:B:286:PRO:HB3	1.95	0.48
1:C:27:VAL:O	1:C:27:VAL:HG22	2.13	0.48
1:C:381:LEU:CD2	1:C:393:LEU:HD21	2.43	0.48
1:C:745:LEU:HD23	1:C:746:ARG:N	2.27	0.48
1:D:149:VAL:HG22	1:D:150:VAL:H	1.76	0.48
1:D:684:THR:O	1:D:684:THR:OG1	2.24	0.48
1:F:65:LYS:HA	1:F:68:THR:HG23	1.96	0.48
1:G:107:VAL:O	1:G:111:ILE:HG12	2.13	0.48
1:G:742:PRO:HG2	1:G:745:LEU:HD12	1.95	0.48
1:H:599:ILE:O	1:H:599:ILE:HG23	2.14	0.48
1:J:360:LEU:HD23	1:J:373:VAL:HG21	1.95	0.48
1:J:373:VAL:O	1:J:377:VAL:HG13	2.13	0.48
1:K:606:MET:CE	1:K:609:LEU:HD13	2.43	0.48
1:L:190:THR:HG1	3:L:902:ADP:PB	2.36	0.48
1:L:465:GLU:CG	1:L:473:LYS:HD3	2.43	0.48
1:B:251:GLN:HG3	1:B:281:PRO:HB3	1.95	0.48
1:B:637:ARG:O	1:B:638:HIS:CG	2.66	0.48
1:C:464:MET:N	1:C:464:MET:SD	2.86	0.48
1:D:531:THR:HG22	1:D:531:THR:O	2.13	0.48
1:E:639:LEU:O	1:E:639:LEU:CD2	2.62	0.48
1:E:735:LEU:CD1	1:E:763:LEU:HD21	2.43	0.48
1:F:34:LEU:HD12	1:F:118:VAL:HG21	1.96	0.48
1:F:169:LEU:CD2	1:F:170:LEU:HG	2.43	0.48
1:F:483:GLU:OE2	1:F:484:PHE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:701:ASP:OD1	1:F:703:LYS:N	2.38	0.48
1:I:701:ASP:OD1	1:I:701:ASP:C	2.52	0.48
1:K:186:GLY:CA	1:K:351:LEU:HD22	2.43	0.48
1:K:429:LEU:HD23	1:K:591:TYR:CE2	2.48	0.48
1:K:717:LEU:HD23	1:K:718:GLU:N	2.29	0.48
1:L:100:HIS:ND1	1:L:104:VAL:HG23	2.27	0.48
1:L:634:GLU:OE1	1:L:634:GLU:N	2.40	0.48
1:L:843:MET:HE3	1:L:878:LEU:CD1	2.43	0.48
1:A:111:ILE:O	1:A:114:ILE:HG22	2.13	0.48
1:A:283:ASN:CG	1:A:283:ASN:O	2.51	0.48
1:A:854:ILE:O	1:A:858:GLN:HG2	2.14	0.48
1:C:262:VAL:O	1:C:289:VAL:HA	2.13	0.48
1:F:169:LEU:HD12	1:F:206:PHE:HE2	1.77	0.48
1:G:612:ILE:HD11	1:G:633:MET:CE	2.43	0.48
1:H:178:VAL:HG21	1:H:302:CYS:HB3	1.95	0.48
1:I:24:ILE:O	1:I:28:LYS:N	2.47	0.48
1:A:501:LEU:HD11	1:A:507:PHE:CZ	2.49	0.48
1:A:544:PHE:CE1	1:A:570:ASP:OD2	2.67	0.48
1:B:100:HIS:O	1:B:100:HIS:ND1	2.46	0.48
1:E:350:PRO:HB3	3:E:902:ADP:C4	2.48	0.48
1:G:52:HIS:O	1:G:59:LEU:HD12	2.13	0.48
1:I:66:ILE:O	1:I:70:VAL:HG23	2.12	0.48
1:I:463:VAL:HG23	1:I:472:ILE:HG23	1.95	0.48
1:J:47:GLN:CB	1:J:132:LEU:HD13	2.43	0.48
1:J:58:VAL:O	1:J:62:LEU:HG	2.14	0.48
1:J:146:LYS:HB3	1:J:147:PRO:HD2	1.96	0.48
1:J:151:GLU:HG3	1:J:152:GLU:HG3	1.94	0.48
1:L:272:ALA:O	1:L:276:ILE:HG22	2.13	0.48
1:A:172:GLU:O	1:A:288:ARG:NH2	2.45	0.48
1:E:254:LEU:C	1:E:254:LEU:HD23	2.34	0.48
1:F:228:ILE:HD11	1:F:250:ILE:HG13	1.94	0.48
1:G:41:PHE:HZ	1:G:122:ARG:HG2	1.79	0.48
1:G:168:ARG:CZ	1:G:307:HIS:HB2	2.44	0.48
1:G:274:GLU:OE1	1:G:277:LYS:NZ	2.29	0.48
1:I:854:ILE:O	1:I:858:GLN:HG2	2.14	0.48
1:J:464:MET:HE1	1:J:476:ARG:HD3	1.96	0.48
1:K:24:ILE:O	1:K:24:ILE:CG2	2.61	0.48
1:K:122:ARG:O	1:K:126:ALA:N	2.47	0.48
1:K:881:PHE:HB3	1:K:882:PRO:HD3	1.94	0.48
1:L:224:PHE:O	1:L:228:ILE:HD12	2.14	0.48
1:A:677:THR:HG22	1:A:678:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LEU:HD12	1:A:779:PHE:CE1	2.48	0.48
1:B:115:ARG:O	1:B:118:VAL:HG22	2.14	0.48
1:B:684:THR:OG1	1:B:687:LEU:HD12	2.13	0.48
1:C:797:TRP:CZ3	1:C:820:VAL:HG21	2.49	0.48
1:E:350:PRO:O	1:E:354:VAL:HG23	2.13	0.48
1:F:100:HIS:CE1	1:F:103:ARG:HG3	2.49	0.48
1:F:398:TYR:HA	1:F:401:LEU:HD23	1.95	0.48
1:J:401:LEU:HB3	1:J:406:LYS:HG3	1.96	0.48
1:J:773:LYS:HG2	1:J:797:TRP:HB3	1.96	0.48
1:A:169:LEU:HD12	1:A:170:LEU:N	2.29	0.48
1:E:539:ARG:O	1:E:566:LEU:HD23	2.14	0.48
1:E:681:PHE:CD1	1:E:714:LEU:HD21	2.46	0.48
1:F:677:THR:OG1	1:F:678:GLU:OE1	2.27	0.48
1:I:875:ALA:HB1	1:I:877:LYS:HZ1	1.79	0.48
1:L:41:PHE:N	1:L:41:PHE:CD1	2.80	0.48
1:A:830:VAL:HG22	1:A:855:SER:OG	2.13	0.48
1:B:677:THR:HG22	1:B:678:GLU:N	2.29	0.48
1:C:202:ILE:HG22	1:C:209:ARG:CD	2.43	0.48
1:E:614:THR:HG22	1:E:615:ILE:N	2.29	0.48
1:H:350:PRO:O	1:H:354:VAL:HG23	2.14	0.48
1:H:505:GLN:OE1	1:H:505:GLN:N	2.45	0.48
1:I:875:ALA:HB1	1:I:877:LYS:CE	2.43	0.48
1:J:350:PRO:HB2	3:J:902:ADP:C8	2.49	0.48
1:K:59:LEU:HA	1:K:62:LEU:HD12	1.95	0.48
1:A:788:GLY:N	1:A:812:ASP:OD1	2.47	0.47
1:B:98:LEU:HB2	1:B:99:PRO:HD3	1.96	0.47
1:B:103:ARG:O	1:B:107:VAL:HG23	2.13	0.47
1:B:676:CYS:O	1:B:677:THR:OG1	2.28	0.47
1:C:178:VAL:CG2	1:C:291:LEU:HD23	2.44	0.47
1:D:592:VAL:O	1:D:592:VAL:HG23	2.14	0.47
1:E:113:ALA:O	1:E:117:LYS:HG3	2.14	0.47
1:E:703:LYS:HG3	1:E:704:SER:N	2.28	0.47
1:E:751:LEU:HD23	1:E:752:ASP:HB2	1.96	0.47
1:F:835:ALA:HB2	1:F:859:ILE:HG23	1.96	0.47
1:G:674:GLU:OE1	1:G:674:GLU:N	2.39	0.47
1:H:409:PHE:HA	1:H:412:CYS:SG	2.54	0.47
1:I:59:LEU:O	1:I:63:VAL:HG13	2.14	0.47
1:A:599:ILE:HG23	1:A:599:ILE:O	2.14	0.47
1:E:714:LEU:HD12	1:E:717:LEU:CD1	2.37	0.47
1:F:66:ILE:O	1:F:70:VAL:HG23	2.14	0.47
1:F:834:LEU:HA	1:F:837:ILE:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:539:ARG:O	1:H:566:LEU:HD23	2.14	0.47
1:H:830:VAL:HG23	1:H:859:ILE:HD11	1.96	0.47
1:I:718:GLU:CG	1:I:718:GLU:O	2.62	0.47
1:J:77:ILE:O	1:J:81:VAL:HG23	2.14	0.47
1:B:507:PHE:CE2	1:B:528:PHE:HA	2.50	0.47
1:C:27:VAL:HG22	1:C:30:ALA:HB3	1.95	0.47
1:D:119:ARG:NE	1:D:123:GLN:OE1	2.33	0.47
1:D:350:PRO:HG2	3:D:902:ADP:C2	2.48	0.47
1:D:641:THR:O	1:D:670:THR:OG1	2.25	0.47
1:G:531:THR:HG22	1:G:531:THR:O	2.12	0.47
1:G:692:ILE:HD13	1:G:699:LEU:HD11	1.96	0.47
1:I:788:GLY:N	1:I:812:ASP:OD1	2.48	0.47
1:I:800:ARG:NH1	1:I:823:CYS:O	2.47	0.47
1:K:107:VAL:O	1:K:111:ILE:CD1	2.53	0.47
1:K:436:ILE:O	1:K:436:ILE:HG22	2.13	0.47
1:L:732:LYS:O	1:L:733:LEU:HD23	2.14	0.47
1:A:78:ASP:O	1:A:82:ILE:HG22	2.14	0.47
1:B:345:LYS:NZ	1:B:374:ASP:OD1	2.44	0.47
1:B:401:LEU:HD23	1:B:406:LYS:HA	1.95	0.47
1:B:681:PHE:HB3	1:B:714:LEU:HD21	1.96	0.47
1:D:854:ILE:O	1:D:858:GLN:HG3	2.14	0.47
1:E:15:GLN:O	1:E:19:ASP:OD2	2.33	0.47
1:E:146:LYS:HB3	1:E:147:PRO:HD2	1.97	0.47
1:F:41:PHE:HZ	1:F:121:ILE:HB	1.79	0.47
1:F:590:ARG:HA	1:F:612:ILE:HA	1.97	0.47
1:F:821:LEU:HD12	1:F:845:LEU:HD21	1.95	0.47
1:G:148:PRO:HD3	1:G:453:ASN:HB3	1.97	0.47
1:H:501:LEU:HD11	1:H:507:PHE:CZ	2.48	0.47
1:H:660:LEU:HD13	1:H:683:ARG:NH2	2.30	0.47
1:J:429:LEU:HD23	1:J:591:TYR:CD2	2.49	0.47
1:J:511:ARG:HB3	1:J:511:ARG:NH1	2.29	0.47
1:K:746:ARG:NE	1:K:770:GLU:OE1	2.47	0.47
1:L:356:ILE:HD11	1:L:393:LEU:HD11	1.96	0.47
1:A:614:THR:HG22	1:A:615:ILE:N	2.29	0.47
1:B:728:ILE:CG1	1:B:730:THR:HG23	2.36	0.47
1:C:350:PRO:HG2	3:C:902:ADP:C8	2.49	0.47
1:D:835:ALA:HB2	1:D:859:ILE:HG23	1.97	0.47
1:E:6:VAL:HG22	1:E:70:VAL:HG21	1.96	0.47
1:F:24:ILE:O	1:F:24:ILE:CG2	2.62	0.47
1:H:677:THR:HG22	1:H:678:GLU:N	2.30	0.47
1:J:274:GLU:HA	1:J:277:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:ILE:O	1:K:81:VAL:HG23	2.14	0.47
1:K:209:ARG:O	1:K:210:ILE:HD13	2.15	0.47
1:L:255:GLY:O	1:L:285:LYS:NZ	2.47	0.47
1:A:844:MET:SD	1:A:881:PHE:HE2	2.38	0.47
1:B:225:LEU:HD23	1:B:225:LEU:O	2.14	0.47
1:C:30:ALA:O	1:C:34:LEU:HG	2.14	0.47
1:D:612:ILE:HD11	1:D:633:MET:CE	2.45	0.47
1:D:717:LEU:HD21	1:D:719:ASN:O	2.14	0.47
1:F:149:VAL:HG22	1:F:150:VAL:N	2.28	0.47
1:G:226:ASN:O	1:G:229:SER:OG	2.30	0.47
1:H:6:VAL:O	1:H:10:VAL:HG23	2.15	0.47
1:I:65:LYS:O	1:I:69:VAL:HG23	2.14	0.47
1:K:334:GLU:OE1	1:K:334:GLU:N	2.39	0.47
1:L:732:LYS:NZ	1:L:780:SER:OG	2.48	0.47
1:A:129:LEU:HD22	1:A:133:GLN:OE1	2.14	0.47
1:A:166:ILE:HG12	1:A:202:ILE:HD11	1.95	0.47
1:A:399:ASP:C	1:A:399:ASP:OD1	2.53	0.47
1:A:702:ASN:C	1:A:704:SER:N	2.68	0.47
1:B:22:GLU:OE1	1:B:22:GLU:N	2.42	0.47
1:B:463:VAL:HG23	1:B:472:ILE:HD11	1.96	0.47
1:B:741:PHE:HD2	1:B:766:LEU:HD11	1.79	0.47
1:C:169:LEU:HD11	1:C:206:PHE:CZ	2.50	0.47
1:C:184:MET:N	1:C:184:MET:SD	2.88	0.47
1:C:751:LEU:HD23	1:C:776:GLU:OE1	2.15	0.47
1:E:82:ILE:HD12	1:E:565:LEU:CD2	2.43	0.47
1:E:409:PHE:CE1	1:E:460:LEU:HB3	2.50	0.47
1:F:97:ASP:O	1:F:101:TYR:HB3	2.14	0.47
1:F:175:HIS:N	1:F:285:LYS:O	2.43	0.47
1:F:345:LYS:CD	1:F:377:VAL:HG13	2.45	0.47
1:F:521:ILE:HD11	1:F:541:PHE:CE1	2.50	0.47
1:G:158:PHE:HE1	1:G:309:LEU:HD11	1.79	0.47
1:H:291:LEU:HD12	1:H:291:LEU:O	2.14	0.47
1:H:416:PRO:HG3	1:H:522:HIS:CG	2.49	0.47
1:J:74:GLU:O	1:J:78:ASP:OD1	2.33	0.47
1:J:120:GLU:O	1:J:124:THR:HG23	2.15	0.47
1:J:234:ASN:OD1	1:J:234:ASN:O	2.33	0.47
1:J:463:VAL:HG21	1:J:472:ILE:HD12	1.97	0.47
1:K:592:VAL:O	1:K:592:VAL:CG1	2.62	0.47
1:L:500:LYS:O	1:L:505:GLN:OE1	2.32	0.47
1:L:866:GLN:O	1:L:871:THR:OG1	2.32	0.47
1:B:590:ARG:HA	1:B:612:ILE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:MET:O	1:B:609:LEU:HD12	2.15	0.47
1:B:752:ASP:OD1	1:B:754:TRP:NE1	2.48	0.47
1:E:413:SER:OG	1:E:496:PHE:HZ	1.98	0.47
1:E:421:ILE:HG21	1:E:426:LEU:HD22	1.96	0.47
1:E:746:ARG:CG	1:E:746:ARG:O	2.62	0.47
1:E:777:ASN:N	1:E:800:ARG:O	2.48	0.47
1:G:98:LEU:HB2	1:G:99:PRO:HD3	1.96	0.47
1:G:508:PRO:HG2	1:G:513:LEU:HD21	1.97	0.47
1:H:415:PHE:CE2	1:H:544:PHE:CZ	3.03	0.47
1:H:837:ILE:O	1:H:863:LYS:NZ	2.46	0.47
1:I:120:GLU:OE1	1:I:121:ILE:HD13	2.15	0.47
1:I:415:PHE:CE2	1:I:421:ILE:HG23	2.49	0.47
1:J:325:VAL:O	1:J:361:ILE:HD11	2.15	0.47
1:J:350:PRO:CB	3:J:902:ADP:C8	2.98	0.47
1:K:660:LEU:HD12	1:K:683:ARG:HH21	1.79	0.47
1:B:6:VAL:O	1:B:10:VAL:HG23	2.14	0.47
1:F:429:LEU:HD23	1:F:591:TYR:CE2	2.50	0.47
1:F:766:LEU:HD13	1:F:769:LEU:HD12	1.97	0.47
1:F:770:GLU:OE1	1:F:794:LEU:HD13	2.15	0.47
1:I:291:LEU:HD12	1:I:291:LEU:O	2.15	0.47
1:J:483:GLU:HG3	1:J:484:PHE:N	2.30	0.47
1:J:499:ILE:O	1:J:499:ILE:CG1	2.63	0.47
1:J:613:GLN:O	1:J:636:LEU:HD12	2.14	0.47
1:K:170:LEU:HD21	1:K:205:GLU:HG2	1.96	0.47
1:L:330:LYS:HA	1:L:330:LYS:HE3	1.97	0.47
1:A:602:LEU:HD21	1:A:617:ILE:HD11	1.97	0.47
1:C:176:LEU:CD2	1:C:282:ASN:HA	2.45	0.47
1:E:429:LEU:O	1:E:430:TRP:C	2.54	0.47
1:E:735:LEU:HD13	1:E:763:LEU:HD21	1.97	0.47
1:F:102:LYS:HA	1:F:105:LYS:HE3	1.97	0.47
1:G:273:TRP:HA	1:G:276:ILE:HG22	1.96	0.47
1:I:254:LEU:HD11	1:I:260:TYR:CB	2.45	0.47
1:K:295:ASP:HB3	1:K:298:VAL:HG22	1.96	0.47
1:K:677:THR:OG1	1:K:678:GLU:OE1	2.33	0.47
1:B:169:LEU:HD11	1:B:170:LEU:HD11	1.97	0.46
1:B:244:GLU:CG	1:C:511:ARG:HH12	2.28	0.46
1:E:432:ALA:O	1:E:590:ARG:NE	2.42	0.46
1:E:507:PHE:CE2	1:E:528:PHE:HA	2.50	0.46
1:E:677:THR:HG22	1:E:678:GLU:N	2.30	0.46
1:H:63:VAL:HA	1:H:66:ILE:HD12	1.96	0.46
1:I:312:LEU:HD12	1:I:316:GLU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:396:MET:O	1:J:400:ARG:NH1	2.48	0.46
1:K:63:VAL:HG23	1:K:67:ARG:HH12	1.79	0.46
1:K:73:ALA:HB2	1:K:114:ILE:HG12	1.97	0.46
1:K:251:GLN:HG2	1:K:281:PRO:HB3	1.96	0.46
1:K:612:ILE:HD11	1:K:633:MET:SD	2.55	0.46
1:L:816:LEU:HD22	1:L:840:PHE:CD1	2.50	0.46
1:B:80:PHE:HB2	1:B:111:ILE:HD11	1.97	0.46
1:B:219:ARG:CD	1:B:222:GLU:OE1	2.63	0.46
1:B:411:TYR:HB2	1:B:435:PHE:HE2	1.80	0.46
1:B:881:PHE:HB2	1:B:882:PRO:HD3	1.98	0.46
1:C:677:THR:HG22	1:C:678:GLU:N	2.30	0.46
1:G:732:LYS:NZ	1:G:780:SER:OG	2.47	0.46
1:H:96:LEU:HD22	1:H:101:TYR:CE2	2.50	0.46
1:H:96:LEU:HD12	1:H:96:LEU:O	2.15	0.46
1:H:178:VAL:O	1:H:303:ASN:ND2	2.49	0.46
1:H:756:GLU:OE1	1:H:756:GLU:N	2.44	0.46
1:I:433:GLU:CD	1:I:568:VAL:HG21	2.35	0.46
1:J:799:GLU:OE1	1:J:822:ILE:HG21	2.14	0.46
1:K:356:ILE:HD11	1:K:393:LEU:HD21	1.97	0.46
1:L:103:ARG:NE	1:L:103:ARG:O	2.48	0.46
1:L:211:TRP:HZ3	1:L:263:VAL:HG11	1.80	0.46
1:B:469:ASP:N	1:B:469:ASP:OD1	2.46	0.46
1:B:607:GLY:HA2	1:B:633:MET:HE2	1.97	0.46
1:D:41:PHE:CZ	1:D:122:ARG:HB2	2.50	0.46
1:E:118:VAL:O	1:E:120:GLU:O	2.34	0.46
1:E:830:VAL:CG2	1:E:859:ILE:HD11	2.45	0.46
1:F:876:PHE:HE1	1:F:878:LEU:HD13	1.80	0.46
1:H:69:VAL:HG23	1:H:114:ILE:HD11	1.97	0.46
1:H:501:LEU:HD11	1:H:507:PHE:CD1	2.50	0.46
1:K:149:VAL:HG22	1:K:150:VAL:N	2.30	0.46
1:K:800:ARG:NE	1:K:800:ARG:HA	2.30	0.46
1:B:233:ARG:HA	1:B:233:ARG:NE	2.31	0.46
1:D:228:ILE:HD11	1:D:250:ILE:HG13	1.97	0.46
1:E:274:GLU:OE1	1:E:274:GLU:HA	2.16	0.46
1:E:295:ASP:OD1	1:E:296:SER:N	2.49	0.46
1:G:478:HIS:HB3	1:G:481:LEU:HD13	1.97	0.46
1:H:684:THR:O	1:H:684:THR:OG1	2.27	0.46
1:J:34:LEU:CD2	1:J:118:VAL:HG21	2.46	0.46
1:B:415:PHE:CE2	1:B:421:ILE:HG23	2.51	0.46
1:C:421:ILE:N	1:C:475:CYS:O	2.41	0.46
1:C:813:PHE:HB3	1:C:816:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:O	3:D:902:ADP:N6	2.48	0.46
1:D:844:MET:SD	1:D:881:PHE:CE1	3.09	0.46
1:E:701:ASP:OD1	1:E:703:LYS:HG2	2.16	0.46
1:H:653:PRO:HD3	1:H:660:LEU:HD11	1.97	0.46
1:J:241:MET:CE	1:J:245:ASP:OD1	2.64	0.46
1:J:274:GLU:HA	1:J:274:GLU:OE1	2.14	0.46
1:K:499:ILE:HD11	1:K:521:ILE:HD12	1.98	0.46
1:K:735:LEU:CD1	1:K:763:LEU:HD21	2.45	0.46
1:L:481:LEU:O	1:L:485:CYS:SG	2.72	0.46
1:B:64:LYS:HD3	1:B:65:LYS:N	2.31	0.46
1:B:211:TRP:CZ3	1:B:263:VAL:HG11	2.50	0.46
1:B:219:ARG:CB	1:B:222:GLU:OE1	2.64	0.46
1:B:421:ILE:HD12	1:B:476:ARG:HA	1.96	0.46
1:C:452:LEU:HD11	1:C:456:ILE:HD11	1.96	0.46
1:C:590:ARG:HA	1:C:612:ILE:HA	1.98	0.46
1:E:74:GLU:O	1:E:78:ASP:OD1	2.33	0.46
1:F:207:PHE:CD1	1:F:883:PRO:HD2	2.51	0.46
1:F:334:GLU:OE1	1:F:334:GLU:N	2.37	0.46
1:F:499:ILE:HD11	1:F:519:LEU:CD1	2.45	0.46
1:F:523:SER:OG	1:F:524:SER:N	2.48	0.46
1:G:390:CYS:O	1:G:394:VAL:HG23	2.15	0.46
1:I:433:GLU:OE2	1:I:568:VAL:HG21	2.15	0.46
1:J:353:ILE:O	1:J:356:ILE:HG22	2.15	0.46
1:K:65:LYS:HA	1:K:68:THR:CG2	2.44	0.46
1:K:108:ALA:HB1	1:K:112:LYS:HE3	1.97	0.46
1:A:58:VAL:O	1:A:62:LEU:HG	2.15	0.46
1:A:260:TYR:OH	1:A:281:PRO:O	2.33	0.46
1:D:401:LEU:HD23	1:D:406:LYS:HA	1.97	0.46
1:E:207:PHE:CD1	1:E:883:PRO:CD	2.98	0.46
1:F:494:ASN:ND2	1:F:494:ASN:C	2.66	0.46
1:F:521:ILE:HD11	1:F:541:PHE:CZ	2.51	0.46
1:G:83:GLU:HG3	1:G:104:VAL:HG22	1.97	0.46
1:H:169:LEU:HD12	1:H:170:LEU:N	2.30	0.46
1:K:56:ASN:CB	1:K:59:LEU:HD22	2.44	0.46
1:K:158:PHE:CE1	1:K:309:LEU:HD11	2.51	0.46
1:L:76:ALA:CB	1:L:111:ILE:HG22	2.46	0.46
1:L:148:PRO:HD3	1:L:453:ASN:HB3	1.98	0.46
1:B:754:TRP:CZ3	1:B:777:ASN:HB3	2.51	0.46
1:C:679:GLU:O	1:C:683:ARG:HG2	2.16	0.46
1:C:797:TRP:NE1	1:C:799:GLU:OE2	2.49	0.46
1:D:467:THR:HG22	2:D:901:IHP:O43	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:LEU:CD1	1:D:717:LEU:HD12	2.46	0.46
1:E:15:GLN:HG2	1:E:19:ASP:OD2	2.16	0.46
1:E:110:GLU:O	1:E:114:ILE:HG12	2.16	0.46
1:F:127:ILE:HD12	1:F:129:LEU:HG	1.97	0.46
1:F:176:LEU:HD13	1:F:260:TYR:OH	2.15	0.46
1:H:838:ARG:NH2	1:H:866:GLN:OE1	2.48	0.46
1:J:295:ASP:OD1	1:J:296:SER:N	2.48	0.46
1:K:645:ALA:O	1:K:672:ALA:N	2.44	0.46
1:D:356:ILE:HD11	1:D:393:LEU:HD11	1.97	0.46
1:F:350:PRO:CB	3:F:902:ADP:C8	2.99	0.46
1:G:601:ILE:HD11	1:G:627:GLN:CD	2.35	0.46
1:G:639:LEU:HD23	1:G:639:LEU:O	2.15	0.46
1:I:27:VAL:O	1:I:27:VAL:CG2	2.64	0.46
1:J:446:CYS:O	1:J:450:ASP:OD2	2.33	0.46
1:K:52:HIS:O	1:K:53:ILE:C	2.52	0.46
1:K:65:LYS:O	1:K:69:VAL:HG23	2.16	0.46
1:K:305:ILE:HG22	1:K:305:ILE:O	2.15	0.46
1:K:429:LEU:HD23	1:K:591:TYR:CD2	2.50	0.46
1:K:717:LEU:HD23	1:K:717:LEU:C	2.36	0.46
1:K:819:LEU:HD23	1:K:843:MET:HE2	1.98	0.46
1:L:592:VAL:O	1:L:592:VAL:HG23	2.15	0.46
1:A:832:ILE:HD12	1:A:859:ILE:HG12	1.97	0.46
1:B:250:ILE:HG21	1:B:279:ALA:HB1	1.98	0.46
1:C:410:LEU:HD23	1:C:489:ALA:HB2	1.97	0.46
1:D:115:ARG:O	1:D:118:VAL:HG22	2.16	0.46
1:D:591:TYR:CD1	1:D:614:THR:HB	2.51	0.46
1:E:73:ALA:HA	1:E:114:ILE:HG21	1.97	0.46
1:E:412:CYS:CB	1:E:477:LEU:HD11	2.46	0.46
1:F:19:ASP:OD1	1:F:20:ASN:N	2.49	0.46
1:G:630:ILE:HD11	1:G:647:LEU:HD12	1.97	0.46
1:G:857:ARG:NH1	1:G:885:LEU:O	2.49	0.46
1:I:409:PHE:CE2	1:I:485:CYS:SG	3.09	0.46
1:J:32:GLU:OE1	1:J:32:GLU:O	2.34	0.46
1:J:507:PHE:CE2	1:J:528:PHE:HA	2.50	0.46
1:J:700:LEU:HD13	1:J:733:LEU:HB3	1.98	0.46
1:J:830:VAL:HG23	1:J:859:ILE:HD11	1.98	0.46
1:K:463:VAL:HG13	1:K:472:ILE:HG13	1.98	0.46
1:C:96:LEU:HD22	1:C:101:TYR:CE2	2.51	0.45
1:C:749:THR:HG23	1:C:773:LYS:HB3	1.97	0.45
1:D:835:ALA:CB	1:D:859:ILE:HG23	2.46	0.45
1:E:16:LEU:HD21	1:E:81:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:GLU:O	1:E:121:ILE:HB	2.17	0.45
1:F:73:ALA:HA	1:F:114:ILE:HD13	1.98	0.45
1:F:75:ASP:OD1	1:F:517:ARG:NH1	2.49	0.45
1:F:592:VAL:O	1:F:592:VAL:CG2	2.62	0.45
1:F:729:GLN:OE1	1:F:754:TRP:CE3	2.68	0.45
1:G:413:SER:CB	1:G:485:CYS:HB3	2.43	0.45
1:I:469:ASP:HB2	1:I:746:ARG:HH22	1.81	0.45
1:J:409:PHE:CE2	1:J:485:CYS:SG	3.08	0.45
1:K:111:ILE:O	1:K:114:ILE:CG2	2.64	0.45
1:L:88:LYS:N	1:L:88:LYS:HD2	2.30	0.45
1:A:450:ASP:O	1:A:454:ASP:OD2	2.35	0.45
1:A:718:GLU:CG	1:A:718:GLU:O	2.65	0.45
1:B:24:ILE:O	1:B:24:ILE:CG2	2.64	0.45
1:B:121:ILE:HA	1:B:124:THR:HG23	1.98	0.45
1:B:295:ASP:OD1	1:B:296:SER:N	2.49	0.45
1:E:11:GLU:OE1	1:E:437:GLN:NE2	2.49	0.45
1:E:27:VAL:HG13	1:E:80:PHE:CE2	2.51	0.45
1:E:630:ILE:HG22	1:E:633:MET:HE3	1.97	0.45
1:E:795:VAL:HG13	1:E:818:HIS:HB3	1.99	0.45
1:E:816:LEU:HD23	1:E:817:LYS:H	1.80	0.45
1:F:186:GLY:O	1:F:351:LEU:HD23	2.16	0.45
1:H:714:LEU:CD1	1:H:717:LEU:HD12	2.45	0.45
1:L:155:VAL:HG13	3:L:902:ADP:C6	2.52	0.45
1:L:223:LEU:HD21	1:L:276:ILE:HD11	1.98	0.45
1:A:34:LEU:HD13	1:A:118:VAL:HG21	1.98	0.45
1:D:360:LEU:HD23	1:D:373:VAL:HG21	1.98	0.45
1:D:413:SER:HB2	1:D:485:CYS:HB2	1.97	0.45
1:E:428:ARG:HH12	1:E:640:HIS:CD2	2.35	0.45
1:F:839:SER:HA	1:F:874:ILE:HD12	1.98	0.45
1:G:501:LEU:HD23	1:G:501:LEU:H	1.81	0.45
1:H:878:LEU:HD12	1:H:879:SER:N	2.31	0.45
1:I:521:ILE:HD11	1:I:541:PHE:CZ	2.51	0.45
1:J:102:LYS:HA	1:J:106:GLU:CB	2.47	0.45
1:K:610:TRP:NE1	1:K:611:ASN:OD1	2.50	0.45
1:A:103:ARG:O	1:A:103:ARG:HD2	2.17	0.45
1:A:297:LYS:O	1:A:301:GLN:NE2	2.50	0.45
1:A:639:LEU:O	1:A:639:LEU:CD2	2.65	0.45
1:B:102:LYS:O	1:B:106:GLU:HG2	2.16	0.45
1:B:614:THR:HG22	1:B:615:ILE:N	2.31	0.45
1:C:407:ALA:O	1:C:408:CYS:HB2	2.17	0.45
1:C:827:LEU:HD21	1:C:830:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLU:OE2	1:D:83:GLU:CA	2.64	0.45
1:D:504:GLU:H	1:D:504:GLU:CD	2.20	0.45
1:D:526:LEU:HD23	1:D:549:ILE:HG21	1.97	0.45
1:E:147:PRO:HA	1:E:148:PRO:HD3	1.86	0.45
1:E:784:TRP:CE3	1:E:806:TRP:CD1	3.04	0.45
1:F:377:VAL:CG1	1:F:378:SER:N	2.78	0.45
1:F:695:LYS:HG3	1:F:698:VAL:HG23	1.97	0.45
1:G:251:GLN:HG3	1:G:281:PRO:HB3	1.99	0.45
1:H:717:LEU:HD23	1:H:717:LEU:C	2.37	0.45
1:I:401:LEU:HG	1:I:402:PRO:HD2	1.98	0.45
1:I:467:THR:HG22	1:I:468:SER:N	2.31	0.45
1:L:114:ILE:HA	1:L:117:LYS:HD3	1.99	0.45
1:L:717:LEU:HD21	1:L:719:ASN:O	2.17	0.45
1:A:732:LYS:NZ	1:A:780:SER:OG	2.49	0.45
1:B:483:GLU:HG3	1:B:484:PHE:N	2.32	0.45
1:C:66:ILE:O	1:C:70:VAL:HG23	2.17	0.45
1:C:150:VAL:HG22	1:C:153:ASP:HB3	1.98	0.45
1:E:531:THR:O	1:E:531:THR:HG22	2.15	0.45
1:G:69:VAL:HG21	1:G:121:ILE:HD11	1.98	0.45
1:G:752:ASP:N	1:G:776:GLU:OE1	2.49	0.45
1:H:610:TRP:CE3	1:H:611:ASN:OD1	2.70	0.45
1:J:746:ARG:CG	1:J:746:ARG:O	2.65	0.45
1:K:354:VAL:HG13	1:K:459:ASN:OD1	2.16	0.45
1:K:750:LEU:CD2	1:K:753:THR:HG21	2.47	0.45
1:L:76:ALA:HB3	1:L:111:ILE:HG22	1.98	0.45
1:D:591:TYR:HE1	1:D:614:THR:HG21	1.80	0.45
1:E:24:ILE:O	1:E:24:ILE:HG22	2.15	0.45
1:E:446:CYS:O	1:E:450:ASP:OD2	2.34	0.45
1:F:467:THR:OG1	1:F:469:ASP:OD1	2.21	0.45
1:J:207:PHE:CD2	1:J:883:PRO:HG2	2.51	0.45
1:J:595:SER:OG	1:J:596:SER:N	2.50	0.45
1:K:381:LEU:HD23	1:K:389:ASN:HB2	1.97	0.45
1:K:837:ILE:O	1:K:863:LYS:NZ	2.27	0.45
1:K:854:ILE:O	1:K:858:GLN:HG2	2.16	0.45
1:L:360:LEU:HD23	1:L:373:VAL:HG21	1.98	0.45
1:L:791:CYS:SG	1:L:792:SER:N	2.90	0.45
1:L:854:ILE:O	1:L:858:GLN:HG3	2.16	0.45
1:B:16:LEU:HD21	1:B:81:VAL:HG21	1.97	0.45
1:B:244:GLU:OE1	1:B:244:GLU:C	2.54	0.45
1:C:843:MET:SD	1:C:878:LEU:HD13	2.57	0.45
1:D:24:ILE:HD11	1:D:31:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:VAL:HG11	1:D:466:ARG:CZ	2.47	0.45
1:E:169:LEU:HB2	1:E:170:LEU:HD12	1.98	0.45
1:E:499:ILE:O	1:E:499:ILE:CG2	2.65	0.45
1:F:40:ASP:OD1	1:F:41:PHE:N	2.50	0.45
1:F:271:GLU:OE1	1:F:271:GLU:N	2.44	0.45
1:F:881:PHE:CD2	1:F:882:PRO:HG3	2.51	0.45
1:H:69:VAL:CG2	1:H:114:ILE:HD11	2.47	0.45
1:I:24:ILE:HG22	1:I:24:ILE:O	2.16	0.45
1:I:250:ILE:HG21	1:I:279:ALA:HB1	1.98	0.45
1:I:399:ASP:OD1	1:I:399:ASP:C	2.55	0.45
1:J:24:ILE:HG22	1:J:24:ILE:O	2.16	0.45
1:J:415:PHE:CE2	1:J:544:PHE:CZ	3.05	0.45
1:K:262:VAL:HG23	1:K:289:VAL:HG22	1.96	0.45
1:A:16:LEU:HD23	1:A:24:ILE:HD12	1.99	0.45
1:A:637:ARG:O	1:A:638:HIS:CG	2.69	0.45
1:B:64:LYS:HE2	1:B:64:LYS:HA	1.98	0.45
1:B:338:SER:HB2	1:B:370:TRP:HE3	1.81	0.45
1:C:746:ARG:HA	1:C:769:LEU:HA	1.99	0.45
1:C:774:MET:SD	1:C:778:GLY:N	2.90	0.45
1:D:735:LEU:HD13	1:D:763:LEU:HD21	1.98	0.45
1:E:23:LEU:HD13	1:E:84:ALA:HB3	1.99	0.45
1:E:681:PHE:CD1	1:E:714:LEU:HD11	2.51	0.45
1:F:835:ALA:CB	1:F:859:ILE:HG23	2.46	0.45
1:J:75:ASP:OD1	1:J:539:ARG:NH2	2.50	0.45
1:J:102:LYS:HG3	1:J:108:ALA:HB3	1.98	0.45
1:K:190:THR:HG22	3:K:902:ADP:O1A	2.16	0.45
1:K:825:ASP:OD1	1:K:826:ASN:N	2.50	0.45
1:A:690:LEU:HB3	1:A:717:LEU:HD11	1.99	0.45
1:A:773:LYS:HG2	1:A:797:TRP:HB3	1.99	0.45
1:C:318:TRP:CZ2	1:C:336:VAL:HG13	2.52	0.45
1:C:825:ASP:OD1	1:C:825:ASP:N	2.40	0.45
1:E:82:ILE:CD1	1:E:565:LEU:HD23	2.47	0.45
1:E:157:GLY:O	1:E:310:LYS:NZ	2.38	0.45
1:E:501:LEU:HD23	1:E:507:PHE:CZ	2.51	0.45
1:F:159:ASP:OD1	1:F:159:ASP:N	2.50	0.45
1:F:178:VAL:HG11	1:F:302:CYS:HB3	1.99	0.45
1:F:305:ILE:O	1:F:305:ILE:HG22	2.15	0.45
1:G:464:MET:CE	1:G:476:ARG:CD	2.95	0.45
1:G:844:MET:SD	1:G:844:MET:C	2.95	0.45
1:I:592:VAL:O	1:I:592:VAL:CG1	2.65	0.45
1:K:860:GLN:OE1	1:K:878:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:409:PHE:CE2	1:L:485:CYS:SG	3.08	0.45
1:L:878:LEU:HD12	1:L:879:SER:N	2.32	0.45
1:D:415:PHE:CE2	1:D:544:PHE:CE1	3.05	0.45
1:G:526:LEU:HD23	1:G:549:ILE:HG21	1.97	0.45
1:G:677:THR:HG22	1:G:678:GLU:N	2.32	0.45
1:H:56:ASN:HB3	1:H:59:LEU:HD21	1.99	0.45
1:I:260:TYR:OH	1:I:287:ASN:ND2	2.50	0.45
1:K:52:HIS:HB2	1:K:55:GLU:CG	2.46	0.45
1:L:154:ASP:N	1:L:154:ASP:OD1	2.50	0.45
1:L:188:GLY:HA2	3:L:902:ADP:H5'1	1.98	0.45
1:A:6:VAL:HG22	1:A:70:VAL:HG21	1.99	0.44
1:B:120:GLU:OE2	1:B:124:THR:CG2	2.65	0.44
1:B:163:ASP:OD1	1:B:164:ILE:N	2.50	0.44
1:B:501:LEU:HD11	1:B:507:PHE:CZ	2.51	0.44
1:C:228:ILE:HG21	1:C:238:TYR:CD2	2.52	0.44
1:C:405:LEU:HD12	1:C:455:LEU:CD2	2.48	0.44
1:F:73:ALA:HB2	1:F:114:ILE:HG21	1.97	0.44
1:F:113:ALA:HB1	1:F:117:LYS:HZ3	1.82	0.44
1:F:703:LYS:HA	1:F:703:LYS:CE	2.39	0.44
1:H:408:CYS:SG	1:H:455:LEU:HD11	2.56	0.44
1:H:660:LEU:HD13	1:H:683:ARG:HH21	1.82	0.44
1:J:6:VAL:HG22	1:J:70:VAL:HG21	1.99	0.44
1:J:10:VAL:O	1:J:14:MET:HG3	2.17	0.44
1:J:596:SER:OG	1:J:597:ASP:N	2.50	0.44
1:K:64:LYS:HZ2	1:K:65:LYS:N	2.09	0.44
1:K:82:ILE:HD12	1:K:565:LEU:CD2	2.46	0.44
1:K:176:LEU:CD1	1:K:260:TYR:OH	2.64	0.44
1:L:843:MET:HE3	1:L:856:ALA:HB1	1.99	0.44
1:C:37:ASP:O	1:C:40:ASP:OD1	2.35	0.44
1:C:149:VAL:HG22	1:C:150:VAL:N	2.32	0.44
1:F:9:LEU:HD23	1:F:70:VAL:HG13	1.99	0.44
1:F:829:GLU:OE1	1:F:830:VAL:O	2.36	0.44
1:G:92:VAL:HG11	1:G:97:ASP:HB2	1.99	0.44
1:I:350:PRO:O	1:I:354:VAL:HG23	2.16	0.44
1:K:145:ARG:NH2	1:K:458:ARG:HE	2.15	0.44
1:K:161:GLU:CG	1:K:310:LYS:HE3	2.47	0.44
1:B:237:GLN:OE1	1:B:238:TYR:HE1	1.93	0.44
1:B:746:ARG:CG	1:B:746:ARG:O	2.65	0.44
1:F:701:ASP:OD1	1:F:701:ASP:C	2.56	0.44
1:G:160:GLU:O	1:G:164:ILE:HG12	2.17	0.44
1:H:113:ALA:O	1:H:117:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:589:LEU:O	1:H:612:ILE:HG23	2.17	0.44
1:I:9:LEU:HD23	1:I:38:LEU:HD21	1.99	0.44
1:I:653:PRO:HD3	1:I:660:LEU:HD11	1.99	0.44
1:K:770:GLU:CG	1:K:794:LEU:CD1	2.95	0.44
1:K:804:VAL:HG22	1:K:826:ASN:CG	2.38	0.44
1:C:251:GLN:HG2	1:C:281:PRO:HB3	1.99	0.44
1:E:120:GLU:O	1:E:121:ILE:CB	2.65	0.44
1:F:38:LEU:CD2	1:F:70:VAL:HG22	2.47	0.44
1:I:59:LEU:O	1:I:62:LEU:HG	2.18	0.44
1:I:595:SER:OG	1:I:596:SER:N	2.50	0.44
1:J:429:LEU:O	1:J:430:TRP:C	2.56	0.44
1:K:34:LEU:O	1:K:38:LEU:HG	2.17	0.44
1:K:401:LEU:HD12	1:K:405:LEU:HB3	1.99	0.44
1:L:59:LEU:HD21	1:L:132:LEU:HD22	1.99	0.44
1:A:41:PHE:HE2	1:A:118:VAL:HG13	1.81	0.44
1:A:411:TYR:OH	1:A:433:GLU:OE2	2.21	0.44
1:B:254:LEU:HD11	1:B:260:TYR:HB3	1.96	0.44
1:C:41:PHE:HZ	1:C:122:ARG:HG2	1.82	0.44
1:E:415:PHE:CG	1:E:421:ILE:HG12	2.53	0.44
1:H:15:GLN:O	1:H:19:ASP:OD1	2.36	0.44
1:H:350:PRO:HB3	3:H:902:ADP:C8	2.52	0.44
1:I:830:VAL:HG23	1:I:859:ILE:HD11	1.99	0.44
1:J:64:LYS:O	1:J:65:LYS:HG2	2.18	0.44
1:J:73:ALA:HA	1:J:114:ILE:HG21	1.98	0.44
1:J:405:LEU:HA	1:J:408:CYS:SG	2.58	0.44
1:K:64:LYS:O	1:K:65:LYS:HB2	2.17	0.44
1:K:721:LYS:HD3	2:K:901:IHP:O35	2.18	0.44
1:L:483:GLU:HG3	1:L:484:PHE:N	2.33	0.44
1:A:350:PRO:HB3	3:A:902:ADP:C4	2.53	0.44
1:D:74:GLU:O	1:D:77:ILE:HG22	2.18	0.44
1:D:525:VAL:HG13	1:D:526:LEU:HD22	1.99	0.44
1:F:801:THR:HG22	1:F:824:CYS:SG	2.58	0.44
1:G:165:VAL:HG22	1:G:307:HIS:ND1	2.33	0.44
1:H:29:GLU:OE1	1:H:29:GLU:N	2.39	0.44
1:I:664:SER:O	1:I:666:GLN:HG2	2.18	0.44
1:J:122:ARG:O	1:J:126:ALA:N	2.35	0.44
1:J:368:ARG:HD3	1:J:372:GLN:HG3	1.99	0.44
1:J:501:LEU:HD21	1:J:507:PHE:CE1	2.53	0.44
1:J:511:ARG:NH1	1:J:511:ARG:CB	2.80	0.44
1:K:770:GLU:HG2	1:K:794:LEU:CD1	2.47	0.44
1:L:27:VAL:CG2	1:L:111:ILE:HD11	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:LYS:O	1:L:106:GLU:HG2	2.17	0.44
1:L:147:PRO:HA	1:L:148:PRO:HD3	1.88	0.44
1:A:69:VAL:HG13	1:A:114:ILE:HD11	2.00	0.44
1:A:115:ARG:NH1	1:A:119:ARG:HB2	2.33	0.44
1:A:168:ARG:HD3	1:A:179:VAL:HG13	2.00	0.44
1:A:222:GLU:OE1	1:A:547:LYS:HG2	2.18	0.44
1:A:797:TRP:CE2	1:A:820:VAL:HG11	2.53	0.44
1:B:296:SER:OG	1:B:297:LYS:NZ	2.34	0.44
1:B:396:MET:O	1:B:400:ARG:NH1	2.51	0.44
1:B:408:CYS:HB3	1:B:430:TRP:CE2	2.53	0.44
1:C:75:ASP:OD2	1:C:517:ARG:NH2	2.51	0.44
1:C:521:ILE:O	1:C:543:SER:HA	2.17	0.44
1:D:429:LEU:HD21	1:D:591:TYR:CE2	2.53	0.44
1:E:262:VAL:HG23	1:E:289:VAL:HG22	1.97	0.44
1:E:613:GLN:O	1:E:636:LEU:HD12	2.17	0.44
1:F:429:LEU:HD23	1:F:591:TYR:CD2	2.52	0.44
1:G:630:ILE:HD11	1:G:647:LEU:CD1	2.48	0.44
1:I:178:VAL:O	1:I:303:ASN:ND2	2.51	0.44
1:I:862:LYS:O	1:I:866:GLN:HG3	2.17	0.44
1:K:111:ILE:O	1:K:114:ILE:HG22	2.18	0.44
1:K:169:LEU:HD13	1:K:170:LEU:HG	1.99	0.44
1:K:766:LEU:CD1	1:K:769:LEU:HD12	2.48	0.44
1:B:27:VAL:HG23	1:B:27:VAL:O	2.17	0.44
1:B:169:LEU:CD1	1:B:170:LEU:CG	2.77	0.44
1:B:584:TYR:CE2	1:B:605:LEU:HB2	2.53	0.44
1:B:595:SER:OG	1:B:596:SER:N	2.51	0.44
1:E:463:VAL:HG23	1:E:472:ILE:HD11	2.00	0.44
1:F:424:TRP:CZ3	1:F:640:HIS:CD2	3.05	0.44
1:F:750:LEU:HD23	1:F:753:THR:HG21	1.99	0.44
1:H:773:LYS:CG	1:H:797:TRP:HB3	2.48	0.44
1:I:449:GLU:O	1:I:453:ASN:OD1	2.36	0.44
1:I:643:SER:O	1:I:670:THR:OG1	2.35	0.44
1:J:377:VAL:HG23	1:J:378:SER:N	2.33	0.44
1:J:606:MET:O	1:J:609:LEU:HD12	2.18	0.44
1:A:169:LEU:HD12	1:A:170:LEU:CB	2.47	0.44
1:A:635:ARG:CZ	1:A:635:ARG:HB2	2.47	0.44
1:B:701:ASP:OD1	1:B:703:LYS:N	2.51	0.44
1:B:795:VAL:HG13	1:B:818:HIS:HB3	2.00	0.44
1:C:570:ASP:C	1:C:570:ASP:OD1	2.57	0.44
1:D:188:GLY:HA3	3:D:902:ADP:H2	1.83	0.44
1:D:355:VAL:HG22	1:D:397:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:ASP:OD1	1:D:527:ASP:N	2.49	0.44
1:F:169:LEU:HD13	1:F:202:ILE:CD1	2.47	0.44
1:I:73:ALA:CA	1:I:114:ILE:HG21	2.48	0.44
1:I:555:ASP:O	1:I:558:THR:OG1	2.29	0.44
1:J:714:LEU:CD1	1:J:717:LEU:HD12	2.47	0.44
1:K:87:HIS:CD2	1:K:97:ASP:HB2	2.53	0.44
1:K:159:ASP:N	1:K:159:ASP:OD1	2.51	0.44
1:L:314:GLU:OE2	1:L:344:LYS:HA	2.17	0.44
1:L:330:LYS:N	1:L:330:LYS:HD2	2.33	0.44
1:L:700:LEU:HB2	1:L:733:LEU:HD13	1.99	0.44
1:A:169:LEU:HD12	1:A:169:LEU:C	2.38	0.43
1:A:291:LEU:HD12	1:A:291:LEU:O	2.18	0.43
1:C:97:ASP:O	1:C:101:TYR:HB3	2.18	0.43
1:F:169:LEU:HD13	1:F:202:ILE:HD13	2.00	0.43
1:G:360:LEU:HD23	1:G:373:VAL:HG21	1.99	0.43
1:H:64:LYS:O	1:H:65:LYS:CB	2.66	0.43
1:I:241:MET:SD	1:I:245:ASP:HB3	2.58	0.43
1:I:424:TRP:CZ3	1:I:640:HIS:CE1	3.06	0.43
1:I:835:ALA:CB	1:I:859:ILE:HG23	2.48	0.43
1:K:57:GLU:CD	1:K:60:ARG:HH22	2.21	0.43
1:L:155:VAL:HG12	1:L:158:PHE:CD2	2.53	0.43
1:L:750:LEU:HD22	1:L:753:THR:HG21	2.00	0.43
1:A:100:HIS:O	1:A:104:VAL:HG23	2.18	0.43
1:A:166:ILE:HG23	1:A:169:LEU:HD23	1.99	0.43
1:A:696:ILE:O	1:A:696:ILE:HG22	2.17	0.43
1:B:219:ARG:NE	1:B:222:GLU:OE1	2.51	0.43
1:B:711:VAL:HG12	1:B:742:PRO:HD3	2.00	0.43
1:C:176:LEU:HG	1:C:282:ASN:HA	1.99	0.43
1:D:83:GLU:OE2	1:D:83:GLU:O	2.35	0.43
1:D:114:ILE:O	1:D:118:VAL:HG13	2.17	0.43
1:D:233:ARG:CZ	1:D:233:ARG:HA	2.48	0.43
1:D:795:VAL:HG13	1:D:818:HIS:HB3	2.00	0.43
1:E:6:VAL:O	1:E:10:VAL:HG23	2.17	0.43
1:E:363:LYS:CE	1:E:400:ARG:HE	2.31	0.43
1:G:169:LEU:HD21	1:G:206:PHE:HE2	1.82	0.43
1:I:33:SER:O	1:I:37:ASP:OD1	2.36	0.43
1:I:467:THR:HG23	2:I:901:IHP:P2	2.58	0.43
1:J:718:GLU:O	1:J:718:GLU:CG	2.66	0.43
1:J:854:ILE:O	1:J:858:GLN:HG3	2.17	0.43
1:K:6:VAL:O	1:K:10:VAL:HG23	2.17	0.43
1:K:410:LEU:HD13	1:K:410:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:844:MET:SD	1:L:844:MET:C	2.97	0.43
1:A:678:GLU:HG3	1:A:679:GLU:N	2.33	0.43
1:B:788:GLY:N	1:B:812:ASP:OD1	2.51	0.43
1:C:2:ALA:O	1:C:6:VAL:HG23	2.18	0.43
1:C:98:LEU:HB2	1:C:99:PRO:HD3	1.99	0.43
1:C:273:TRP:CZ2	1:C:277:LYS:HD2	2.52	0.43
1:C:350:PRO:HA	1:C:353:ILE:HD12	1.99	0.43
1:D:219:ARG:HA	1:D:219:ARG:NE	2.33	0.43
1:D:350:PRO:CB	3:D:902:ADP:N3	2.82	0.43
1:D:464:MET:SD	1:D:476:ARG:HD3	2.57	0.43
1:E:65:LYS:HA	1:E:68:THR:HG23	2.00	0.43
1:E:101:TYR:HA	1:E:104:VAL:HG12	1.99	0.43
1:E:584:TYR:CD2	1:E:605:LEU:HB2	2.53	0.43
1:F:57:GLU:HG2	1:F:60:ARG:HH12	1.82	0.43
1:J:369:GLU:O	1:J:373:VAL:HG23	2.18	0.43
1:J:644:SER:O	1:J:644:SER:OG	2.33	0.43
1:J:741:PHE:HD2	1:J:766:LEU:HD11	1.82	0.43
1:K:115:ARG:HD2	1:K:115:ARG:C	2.39	0.43
1:K:214:VAL:O	1:K:266:ASP:O	2.35	0.43
1:L:223:LEU:CD2	1:L:276:ILE:HD11	2.48	0.43
1:A:190:THR:HG22	3:A:902:ADP:O2B	2.18	0.43
1:A:216:GLN:CD	1:A:216:GLN:C	2.77	0.43
1:A:325:VAL:HG13	1:A:326:PHE:CD2	2.53	0.43
1:A:660:LEU:HD13	1:A:683:ARG:HH21	1.83	0.43
1:B:531:THR:HG22	1:B:531:THR:O	2.19	0.43
1:C:151:GLU:HG3	1:C:152:GLU:CG	2.44	0.43
1:C:260:TYR:CE2	1:C:287:ASN:OD1	2.72	0.43
1:C:638:HIS:HB3	1:C:640:HIS:NE2	2.33	0.43
1:C:845:LEU:HB2	1:C:880:ILE:HG22	2.00	0.43
1:E:114:ILE:HD13	1:E:117:LYS:HE2	2.01	0.43
1:E:776:GLU:OE1	1:E:776:GLU:O	2.36	0.43
1:F:6:VAL:O	1:F:10:VAL:HG23	2.18	0.43
1:G:2:ALA:O	1:G:6:VAL:HG23	2.18	0.43
1:G:103:ARG:O	1:G:103:ARG:HD3	2.18	0.43
1:G:237:GLN:OE1	1:G:237:GLN:N	2.46	0.43
1:H:111:ILE:HA	1:H:114:ILE:HG22	2.00	0.43
1:H:283:ASN:O	1:H:283:ASN:CG	2.57	0.43
1:J:41:PHE:N	1:J:41:PHE:CD1	2.85	0.43
1:J:499:ILE:HD11	1:J:521:ILE:HD13	2.00	0.43
1:L:27:VAL:HG11	1:L:111:ILE:CD1	2.47	0.43
1:A:254:LEU:HD11	1:A:260:TYR:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLN:HG2	1:B:19:ASP:OD2	2.18	0.43
1:C:390:CYS:O	1:C:394:VAL:HG23	2.19	0.43
1:C:831:PRO:O	1:C:859:ILE:HD11	2.19	0.43
1:C:835:ALA:HB2	1:C:859:ILE:HG23	2.01	0.43
1:D:177:GLU:H	1:D:288:ARG:HE	1.67	0.43
1:D:350:PRO:HA	1:D:353:ILE:HD12	2.00	0.43
1:F:194:ASN:OD1	1:F:198:LYS:NZ	2.39	0.43
1:F:714:LEU:CD1	1:F:717:LEU:HD12	2.48	0.43
1:H:69:VAL:HG23	1:H:114:ILE:CD1	2.49	0.43
1:H:166:ILE:O	1:H:169:LEU:HB3	2.17	0.43
1:H:241:MET:HE3	1:H:245:ASP:HB3	2.01	0.43
1:I:467:THR:HG23	2:I:901:IHP:O42	2.18	0.43
1:K:11:GLU:CD	1:K:11:GLU:C	2.77	0.43
1:A:595:SER:OG	1:A:596:SER:N	2.52	0.43
1:A:729:GLN:OE1	1:A:754:TRP:CD2	2.71	0.43
1:B:353:ILE:O	1:B:356:ILE:HG22	2.18	0.43
1:B:639:LEU:HD23	1:B:639:LEU:C	2.38	0.43
1:C:64:LYS:O	1:C:65:LYS:HB3	2.18	0.43
1:C:152:GLU:HB3	1:C:323:LYS:HB3	1.99	0.43
1:C:394:VAL:HG21	1:C:481:LEU:HD23	1.99	0.43
1:D:81:VAL:HG13	1:D:588:HIS:CE1	2.54	0.43
1:F:644:SER:O	1:F:644:SER:OG	2.30	0.43
1:F:823:CYS:HA	1:F:847:ASN:HB2	2.00	0.43
1:G:223:LEU:HD22	1:G:276:ILE:HD11	2.00	0.43
1:H:21:VAL:O	1:H:25:SER:N	2.52	0.43
1:H:87:HIS:O	1:H:90:LYS:HB2	2.19	0.43
1:H:408:CYS:SG	1:H:430:TRP:HZ2	2.41	0.43
1:I:732:LYS:NZ	1:I:780:SER:OG	2.51	0.43
1:J:102:LYS:CA	1:J:106:GLU:HB3	2.49	0.43
1:J:105:LYS:HG3	1:J:106:GLU:N	2.32	0.43
1:J:106:GLU:O	1:J:107:VAL:HG12	2.18	0.43
1:J:458:ARG:O	1:J:459:ASN:HB2	2.19	0.43
1:K:445:GLU:O	1:K:449:GLU:HG3	2.19	0.43
1:K:772:LEU:HD12	1:K:773:LYS:N	2.34	0.43
1:L:413:SER:HB2	1:L:485:CYS:HB2	2.00	0.43
1:L:467:THR:OG1	1:L:469:ASP:OD1	2.20	0.43
1:B:405:LEU:HD22	1:B:455:LEU:HG	2.01	0.43
1:B:613:GLN:O	1:B:636:LEU:HD12	2.19	0.43
1:B:680:VAL:O	1:B:684:THR:HG23	2.18	0.43
1:C:261:LEU:HD12	1:C:288:ARG:O	2.19	0.43
1:C:486:ARG:HG2	1:C:486:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:LEU:CD2	1:E:406:LYS:N	2.82	0.43
1:G:76:ALA:HB1	1:G:111:ILE:HG23	2.01	0.43
1:G:436:ILE:O	1:G:436:ILE:HG22	2.19	0.43
1:G:665:LEU:HD23	1:G:666:GLN:N	2.34	0.43
1:H:254:LEU:HD22	1:H:260:TYR:CD2	2.54	0.43
1:H:838:ARG:HA	1:H:838:ARG:NE	2.33	0.43
1:I:154:ASP:N	1:I:154:ASP:OD1	2.51	0.43
1:I:172:GLU:OE1	1:I:175:HIS:ND1	2.52	0.43
1:I:639:LEU:HD23	1:I:639:LEU:C	2.38	0.43
1:J:27:VAL:HG23	1:J:27:VAL:O	2.18	0.43
1:K:354:VAL:HG21	3:K:902:ADP:C8	2.53	0.43
1:L:309:LEU:HD12	1:L:310:LYS:H	1.84	0.43
1:A:602:LEU:HD11	1:A:617:ILE:HD13	2.01	0.43
1:B:262:VAL:HG22	1:B:289:VAL:HG22	2.00	0.43
1:B:273:TRP:HA	1:B:276:ILE:HG22	2.01	0.43
1:D:757:TRP:CE2	1:D:803:LEU:HD13	2.53	0.43
1:E:526:LEU:HG	1:E:549:ILE:HG21	2.01	0.43
1:F:584:TYR:OH	1:F:603:PRO:HG3	2.19	0.43
1:F:596:SER:HB3	1:F:599:ILE:HG22	2.00	0.43
1:I:82:ILE:HD12	1:I:565:LEU:HD22	2.01	0.43
1:I:698:VAL:O	1:I:704:SER:OG	2.36	0.43
1:J:241:MET:HE3	1:J:245:ASP:CB	2.49	0.43
1:J:539:ARG:O	1:J:566:LEU:HD23	2.19	0.43
1:K:351:LEU:HD12	1:K:351:LEU:HA	1.90	0.43
1:B:480:MET:O	1:B:483:GLU:HG3	2.18	0.43
1:C:264:LEU:O	1:C:291:LEU:HA	2.19	0.43
1:D:59:LEU:HA	1:D:62:LEU:HG	2.01	0.43
1:D:614:THR:HG22	1:D:615:ILE:N	2.34	0.43
1:D:630:ILE:HD11	1:D:647:LEU:HD12	1.99	0.43
1:F:37:ASP:HA	1:F:40:ASP:OD2	2.18	0.43
1:F:169:LEU:CG	1:F:170:LEU:HG	2.49	0.43
1:H:467:THR:HG23	2:H:901:IHP:O35	2.19	0.43
1:H:624:LEU:HD12	1:H:625:ASP:H	1.83	0.43
1:H:671:ILE:HD11	1:H:675:SER:O	2.19	0.43
1:I:102:LYS:O	1:I:106:GLU:HG2	2.19	0.43
1:I:794:LEU:HD13	1:I:817:LYS:HB2	2.00	0.43
1:J:314:GLU:OE1	1:J:344:LYS:HD3	2.19	0.43
1:K:771:VAL:HG22	1:K:795:VAL:CG1	2.49	0.43
1:A:105:LYS:O	1:A:108:ALA:HB3	2.18	0.43
1:B:219:ARG:HD2	1:B:222:GLU:OE1	2.19	0.43
1:B:539:ARG:HD2	1:B:565:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:VAL:HG23	1:C:307:HIS:CE1	2.54	0.43
1:C:264:LEU:HD11	1:C:280:PHE:CZ	2.53	0.43
1:C:342:ILE:HG21	1:C:356:ILE:HG21	2.00	0.43
1:D:251:GLN:HG3	1:D:281:PRO:HB3	2.00	0.43
1:D:469:ASP:OD1	1:D:469:ASP:N	2.46	0.43
1:E:2:ALA:HB2	1:E:67:ARG:NE	2.34	0.43
1:E:262:VAL:HG22	1:E:289:VAL:HG22	1.97	0.43
1:G:263:VAL:HG22	1:G:290:LEU:HB3	2.00	0.43
1:G:614:THR:HG22	1:G:615:ILE:N	2.34	0.43
1:H:197:TYR:O	1:H:209:ARG:NH1	2.51	0.43
1:H:729:GLN:OE1	1:H:754:TRP:CD2	2.72	0.43
1:I:409:PHE:CE1	1:I:460:LEU:HB3	2.54	0.43
1:I:832:ILE:HD11	1:I:862:LYS:HD3	2.01	0.43
1:J:74:GLU:OE2	1:J:567:ARG:NH2	2.51	0.43
1:J:211:TRP:CZ3	1:J:263:VAL:HG11	2.54	0.43
1:J:795:VAL:HG13	1:J:818:HIS:HB3	2.01	0.43
1:A:860:GLN:OE1	1:A:878:LEU:HD23	2.18	0.42
1:B:354:VAL:CG1	1:B:459:ASN:HB3	2.49	0.42
1:B:567:ARG:HA	1:B:588:HIS:O	2.19	0.42
1:C:75:ASP:OD2	1:C:537:HIS:ND1	2.52	0.42
1:C:753:THR:OG1	1:C:778:GLY:O	2.37	0.42
1:G:174:ASN:ND2	1:G:284:ASN:O	2.52	0.42
1:G:716:TYR:O	1:G:718:GLU:OE2	2.37	0.42
1:H:254:LEU:HD22	1:H:260:TYR:CG	2.54	0.42
1:I:28:LYS:O	1:I:32:GLU:HG3	2.19	0.42
1:I:209:ARG:O	1:I:210:ILE:HD13	2.18	0.42
1:I:409:PHE:HA	1:I:412:CYS:SG	2.58	0.42
1:L:273:TRP:HA	1:L:276:ILE:HG22	2.00	0.42
1:A:69:VAL:CG1	1:A:118:VAL:HG22	2.49	0.42
1:A:117:LYS:O	1:A:121:ILE:HG12	2.19	0.42
1:A:702:ASN:HA	1:A:705:ALA:CB	2.43	0.42
1:B:244:GLU:C	1:B:244:GLU:CD	2.77	0.42
1:B:816:LEU:HD23	1:B:817:LYS:H	1.83	0.42
1:C:618:ASN:HA	1:C:642:ASN:CG	2.40	0.42
1:D:521:ILE:HG21	1:D:525:VAL:HG23	2.01	0.42
1:E:119:ARG:CZ	1:E:123:GLN:OE1	2.67	0.42
1:E:120:GLU:CD	1:E:121:ILE:N	2.72	0.42
1:E:228:ILE:HD12	1:E:246:LEU:HD13	2.01	0.42
1:E:394:VAL:HG13	1:E:484:PHE:CE1	2.54	0.42
1:G:229:SER:O	1:G:233:ARG:NH2	2.52	0.42
1:G:401:LEU:HD23	1:G:406:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:521:ILE:HG21	1:G:525:VAL:HG23	2.02	0.42
1:G:795:VAL:HG22	1:G:818:HIS:HB3	2.00	0.42
1:I:599:ILE:O	1:I:599:ILE:HG23	2.18	0.42
1:J:511:ARG:HB3	1:J:511:ARG:CZ	2.49	0.42
1:J:630:ILE:HG22	1:J:633:MET:HE3	2.01	0.42
1:K:292:THR:OG1	1:K:292:THR:O	2.37	0.42
1:L:714:LEU:HD12	1:L:717:LEU:HD12	2.01	0.42
1:A:80:PHE:HD1	1:A:80:PHE:O	2.02	0.42
1:A:531:THR:O	1:A:531:THR:HG22	2.19	0.42
1:A:806:TRP:O	1:A:831:PRO:HG3	2.19	0.42
1:C:6:VAL:HG21	1:C:45:LEU:HD11	2.02	0.42
1:C:218:TYR:OH	1:C:275:ARG:NH2	2.51	0.42
1:C:266:ASP:N	1:C:292:THR:O	2.53	0.42
1:C:483:GLU:HB2	1:C:486:ARG:NH2	2.35	0.42
1:C:549:ILE:O	1:C:575:ASN:N	2.45	0.42
1:D:639:LEU:O	1:D:639:LEU:HD23	2.19	0.42
1:F:241:MET:CB	1:F:245:ASP:OD2	2.67	0.42
1:G:51:CYS:HB2	1:G:59:LEU:HD11	2.01	0.42
1:G:74:GLU:O	1:G:75:ASP:C	2.57	0.42
1:H:62:LEU:HD12	1:H:62:LEU:O	2.19	0.42
1:H:531:THR:O	1:H:531:THR:HG22	2.18	0.42
1:J:788:GLY:N	1:J:812:ASP:OD1	2.53	0.42
1:K:101:TYR:CG	1:K:102:LYS:N	2.86	0.42
1:K:104:VAL:O	1:K:107:VAL:HG22	2.19	0.42
1:K:401:LEU:HB2	1:K:406:LYS:HE2	2.01	0.42
1:L:504:GLU:HA	1:L:506:TYR:OH	2.19	0.42
1:L:614:THR:HG22	1:L:615:ILE:N	2.34	0.42
1:L:782:GLU:N	1:L:782:GLU:CD	2.73	0.42
1:B:60:ARG:HA	1:B:63:VAL:HG22	2.00	0.42
1:B:424:TRP:CZ3	1:B:640:HIS:CE1	3.07	0.42
1:B:795:VAL:HG22	1:B:818:HIS:HB3	2.01	0.42
1:C:210:ILE:HD11	1:C:254:LEU:HD21	2.01	0.42
1:C:416:PRO:HD2	1:C:544:PHE:CD2	2.55	0.42
1:D:42:ASN:HA	1:D:45:LEU:HD12	2.02	0.42
1:D:508:PRO:HG2	1:D:513:LEU:HD11	2.00	0.42
1:D:844:MET:SD	1:D:881:PHE:HE1	2.42	0.42
1:E:630:ILE:HA	1:E:633:MET:HE3	2.01	0.42
1:E:681:PHE:HE1	1:E:690:LEU:HD22	1.85	0.42
1:E:788:GLY:N	1:E:812:ASP:OD1	2.52	0.42
1:F:75:ASP:OD1	1:F:517:ARG:NH2	2.51	0.42
1:F:596:SER:O	1:F:619:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:832:ILE:O	1:F:835:ALA:N	2.52	0.42
1:G:83:GLU:OE1	1:G:104:VAL:CG2	2.66	0.42
1:H:664:SER:O	1:H:666:GLN:HG2	2.19	0.42
1:J:464:MET:CE	1:J:476:ARG:HD3	2.49	0.42
1:K:98:LEU:HB2	1:K:99:PRO:HD3	2.01	0.42
1:K:415:PHE:CE2	1:K:544:PHE:CE1	3.08	0.42
1:K:857:ARG:O	1:K:857:ARG:HD3	2.20	0.42
1:L:153:ASP:OD1	1:L:154:ASP:N	2.52	0.42
1:L:527:ASP:N	1:L:527:ASP:OD1	2.52	0.42
1:L:601:ILE:HD11	1:L:627:GLN:CD	2.40	0.42
1:L:843:MET:CE	1:L:856:ALA:HB1	2.49	0.42
1:A:433:GLU:CD	1:A:568:VAL:HG21	2.39	0.42
1:B:592:VAL:O	1:B:592:VAL:CG1	2.66	0.42
1:C:697:SER:OG	1:C:733:LEU:HD11	2.20	0.42
1:E:57:GLU:HA	1:E:60:ARG:CZ	2.50	0.42
1:E:236:LYS:O	1:E:239:HIS:HB2	2.20	0.42
1:F:599:ILE:HG23	1:F:599:ILE:O	2.19	0.42
1:H:120:GLU:OE2	1:H:120:GLU:C	2.57	0.42
1:I:24:ILE:HG23	1:I:27:VAL:HG13	2.01	0.42
1:I:325:VAL:HG13	1:I:326:PHE:N	2.34	0.42
1:J:844:MET:SD	1:J:844:MET:C	2.98	0.42
1:L:96:LEU:HD22	1:L:105:LYS:HZ1	1.84	0.42
1:L:221:ARG:HD2	1:L:243:GLU:HG2	2.01	0.42
1:A:714:LEU:HD12	1:A:717:LEU:CD1	2.49	0.42
1:B:97:ASP:O	1:B:101:TYR:HB3	2.19	0.42
1:B:687:LEU:HD23	1:B:689:LYS:H	1.85	0.42
1:C:178:VAL:HG22	1:C:291:LEU:HD23	2.01	0.42
1:C:399:ASP:OD1	1:C:400:ARG:N	2.53	0.42
1:D:37:ASP:OD1	1:D:119:ARG:NH1	2.53	0.42
1:D:413:SER:HB3	1:D:485:CYS:HB2	2.01	0.42
1:E:22:GLU:OE1	1:E:22:GLU:N	2.43	0.42
1:E:416:PRO:CG	1:E:544:PHE:HB2	2.49	0.42
1:F:345:LYS:HD2	1:F:377:VAL:CG1	2.49	0.42
1:F:735:LEU:HD11	1:F:763:LEU:HD21	2.00	0.42
1:F:803:LEU:O	1:F:827:LEU:N	2.52	0.42
1:G:60:ARG:HD2	1:G:60:ARG:HA	1.94	0.42
1:G:66:ILE:O	1:G:70:VAL:HG12	2.20	0.42
1:H:161:GLU:OE1	1:H:307:HIS:NE2	2.52	0.42
1:H:776:GLU:N	1:H:799:GLU:OE2	2.52	0.42
1:H:797:TRP:CE2	1:H:820:VAL:HG11	2.54	0.42
1:I:85:LYS:HE3	1:I:610:TRP:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:729:GLN:OE1	1:I:754:TRP:CD2	2.73	0.42
1:I:829:GLU:OE1	1:I:829:GLU:CA	2.67	0.42
1:J:584:TYR:OH	1:J:603:PRO:HG2	2.19	0.42
1:L:166:ILE:O	1:L:169:LEU:HB3	2.19	0.42
1:A:190:THR:HG22	3:A:902:ADP:PB	2.60	0.42
1:A:838:ARG:NE	1:A:838:ARG:HA	2.34	0.42
1:B:728:ILE:HG13	1:B:728:ILE:O	2.20	0.42
1:C:745:LEU:HD21	1:C:747:LYS:O	2.19	0.42
1:E:80:PHE:CD1	1:E:80:PHE:O	2.73	0.42
1:E:677:THR:HG22	1:E:678:GLU:H	1.85	0.42
1:F:596:SER:HB3	1:F:599:ILE:CG2	2.50	0.42
1:G:154:ASP:N	1:G:154:ASP:OD1	2.53	0.42
1:G:237:GLN:O	1:G:241:MET:HG3	2.20	0.42
1:G:525:VAL:HG13	1:G:526:LEU:HD22	2.02	0.42
1:G:843:MET:CE	1:G:878:LEU:HD13	2.50	0.42
1:I:176:LEU:HA	1:I:287:ASN:OD1	2.20	0.42
1:I:875:ALA:HB1	1:I:877:LYS:NZ	2.34	0.42
1:J:350:PRO:O	1:J:354:VAL:HG23	2.19	0.42
1:J:429:LEU:O	1:J:432:ALA:N	2.53	0.42
1:K:262:VAL:HG23	1:K:289:VAL:HG13	2.00	0.42
1:L:96:LEU:HD22	1:L:105:LYS:NZ	2.34	0.42
1:L:592:VAL:O	1:L:592:VAL:CG2	2.68	0.42
1:L:843:MET:HE2	1:L:843:MET:HB3	1.85	0.42
1:B:228:ILE:HD13	1:B:238:TYR:CD2	2.54	0.42
1:B:234:ASN:OD1	1:B:234:ASN:O	2.37	0.42
1:B:346:CYS:O	1:B:347:LYS:HB2	2.20	0.42
1:C:23:LEU:HD13	1:C:84:ALA:HB3	2.02	0.42
1:C:404:ASP:O	1:C:407:ALA:HB3	2.19	0.42
1:C:501:LEU:HD13	1:C:507:PHE:CE1	2.55	0.42
1:C:575:ASN:C	1:C:575:ASN:OD1	2.58	0.42
1:E:410:LEU:HB3	1:E:489:ALA:HB2	2.01	0.42
1:F:56:ASN:O	1:F:60:ARG:HG3	2.20	0.42
1:F:377:VAL:HG22	1:F:381:LEU:HD12	2.02	0.42
1:F:819:LEU:HB3	1:F:843:MET:HB2	2.01	0.42
1:H:464:MET:CE	1:H:476:ARG:CD	2.97	0.42
1:H:755:LEU:HB2	1:H:779:PHE:CD1	2.54	0.42
1:H:830:VAL:HG23	1:H:830:VAL:O	2.20	0.42
1:I:158:PHE:HE1	1:I:309:LEU:HD11	1.85	0.42
1:J:408:CYS:HB3	1:J:430:TRP:CE2	2.55	0.42
1:J:433:GLU:CD	1:J:568:VAL:HG21	2.39	0.42
1:K:804:VAL:HG22	1:K:826:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:TYR:CG	1:L:102:LYS:N	2.88	0.42
1:L:158:PHE:CE1	1:L:309:LEU:HD11	2.46	0.42
1:A:425:LYS:HZ1	1:A:616:ILE:HD13	1.84	0.42
1:B:630:ILE:H	1:B:630:ILE:HG12	1.68	0.42
1:B:799:GLU:OE1	1:B:822:ILE:HG21	2.19	0.42
1:D:146:LYS:C	1:D:148:PRO:HD3	2.40	0.42
1:D:717:LEU:HD23	1:D:718:GLU:N	2.35	0.42
1:E:291:LEU:C	1:E:291:LEU:HD12	2.40	0.42
1:E:755:LEU:HB2	1:E:779:PHE:CE1	2.53	0.42
1:G:169:LEU:HD21	1:G:206:PHE:CE2	2.55	0.42
1:H:169:LEU:CD1	1:H:206:PHE:CZ	3.03	0.42
1:I:219:ARG:NH1	1:I:222:GLU:OE2	2.52	0.42
1:I:345:LYS:HZ3	1:I:378:SER:HB3	1.84	0.42
1:I:632:ASN:O	1:I:634:GLU:OE1	2.37	0.42
1:K:16:LEU:HG	1:K:24:ILE:HD12	2.01	0.42
1:K:401:LEU:HB2	1:K:406:LYS:HG2	2.02	0.42
1:K:401:LEU:CB	1:K:406:LYS:HG2	2.49	0.42
1:L:373:VAL:O	1:L:377:VAL:HG23	2.20	0.42
1:L:401:LEU:HG	1:L:402:PRO:HD2	2.02	0.42
1:L:439:LYS:O	1:L:439:LYS:CG	2.68	0.42
1:L:714:LEU:CD1	1:L:717:LEU:HD12	2.50	0.42
1:L:735:LEU:CD1	1:L:763:LEU:HD21	2.50	0.42
1:A:681:PHE:CD1	1:A:714:LEU:HD11	2.54	0.42
1:B:679:GLU:O	1:B:683:ARG:HG2	2.20	0.42
1:C:69:VAL:HG22	1:C:117:LYS:HE3	2.02	0.42
1:C:208:THR:O	1:C:260:TYR:HA	2.20	0.42
1:C:819:LEU:HD12	1:C:820:VAL:N	2.34	0.42
1:C:821:LEU:HB3	1:C:845:LEU:HD23	2.02	0.42
1:D:41:PHE:CE2	1:D:122:ARG:HG3	2.55	0.42
1:D:498:GLU:OE2	1:D:522:HIS:ND1	2.49	0.42
1:E:354:VAL:CG1	1:E:459:ASN:HB3	2.50	0.42
1:E:521:ILE:HG23	1:E:521:ILE:O	2.20	0.42
1:F:59:LEU:HD23	1:F:60:ARG:HG3	2.02	0.42
1:F:67:ARG:HB2	1:F:67:ARG:HH11	1.85	0.42
1:F:166:ILE:O	1:F:169:LEU:HB3	2.20	0.42
1:F:172:GLU:O	1:F:172:GLU:HG3	2.20	0.42
1:G:73:ALA:HA	1:G:114:ILE:HD13	2.02	0.42
1:G:79:LYS:NZ	1:G:536:GLU:OE2	2.38	0.42
1:G:147:PRO:HA	1:G:148:PRO:HD3	1.90	0.42
1:G:544:PHE:CE1	1:G:570:ASP:OD2	2.73	0.42
1:H:60:ARG:HA	1:H:63:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:875:ALA:HB1	1:H:877:LYS:CE	2.50	0.42
1:I:777:ASN:N	1:I:800:ARG:O	2.52	0.42
1:J:169:LEU:HD12	1:J:170:LEU:CG	2.48	0.42
1:J:405:LEU:HA	1:J:405:LEU:HD23	1.94	0.42
1:K:97:ASP:O	1:K:101:TYR:HB3	2.20	0.42
1:L:251:GLN:HG3	1:L:281:PRO:HB3	2.02	0.42
1:L:410:LEU:HB3	1:L:489:ALA:HB2	2.01	0.42
1:L:535:ALA:O	1:L:562:GLY:O	2.37	0.42
1:L:590:ARG:HA	1:L:612:ILE:HA	2.02	0.42
1:L:752:ASP:N	1:L:776:GLU:OE1	2.53	0.42
1:L:845:LEU:CD1	1:L:848:SER:HB2	2.45	0.42
1:L:853:ALA:HB2	1:L:885:LEU:HB3	2.02	0.42
1:A:225:LEU:HD22	1:A:246:LEU:HD13	2.02	0.41
1:B:228:ILE:HG13	1:B:250:ILE:HG13	2.01	0.41
1:B:575:ASN:C	1:B:575:ASN:OD1	2.57	0.41
1:B:853:ALA:HB2	1:B:885:LEU:HB3	2.00	0.41
1:C:499:ILE:HG22	1:C:501:LEU:HD11	2.02	0.41
1:D:34:LEU:HD12	1:D:118:VAL:HG21	2.02	0.41
1:D:732:LYS:NZ	1:D:780:SER:OG	2.52	0.41
1:E:273:TRP:HA	1:E:276:ILE:HG22	2.02	0.41
1:E:612:ILE:HD12	1:E:615:ILE:HD11	2.00	0.41
1:F:114:ILE:HA	1:F:117:LYS:HE2	2.02	0.41
1:G:40:ASP:OD1	1:G:41:PHE:N	2.53	0.41
1:G:878:LEU:HD12	1:G:879:SER:N	2.35	0.41
1:H:163:ASP:O	1:H:167:ASN:OD1	2.38	0.41
1:H:781:GLY:O	1:H:803:LEU:HD12	2.20	0.41
1:I:409:PHE:C	1:I:412:CYS:SG	2.99	0.41
1:J:816:LEU:HD23	1:J:817:LYS:H	1.85	0.41
1:K:108:ALA:HB1	1:K:112:LYS:NZ	2.35	0.41
1:K:426:LEU:HG	1:K:430:TRP:CZ2	2.55	0.41
1:K:750:LEU:HD23	1:K:753:THR:HG21	2.02	0.41
1:B:80:PHE:CD1	1:B:80:PHE:O	2.73	0.41
1:B:103:ARG:CZ	1:B:106:GLU:HB2	2.50	0.41
1:B:119:ARG:O	1:B:123:GLN:HG2	2.20	0.41
1:C:821:LEU:C	1:C:822:ILE:HD13	2.40	0.41
1:D:592:VAL:O	1:D:592:VAL:CG2	2.68	0.41
1:E:36:GLN:O	1:E:40:ASP:OD1	2.38	0.41
1:H:66:ILE:O	1:H:69:VAL:HG12	2.19	0.41
1:H:678:GLU:HG3	1:H:679:GLU:N	2.35	0.41
1:I:813:PHE:O	1:I:837:ILE:HD13	2.20	0.41
1:J:169:LEU:O	1:J:170:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:ARG:HA	1:J:261:LEU:O	2.20	0.41
1:J:464:MET:SD	1:J:476:ARG:HG2	2.60	0.41
1:J:640:HIS:CD2	1:J:640:HIS:N	2.89	0.41
1:J:776:GLU:O	1:J:776:GLU:OE1	2.38	0.41
1:J:857:ARG:NH2	1:J:885:LEU:OXT	2.54	0.41
1:K:52:HIS:C	1:K:54:ASN:N	2.72	0.41
1:L:37:ASP:HB3	1:L:41:PHE:CE2	2.55	0.41
1:L:647:LEU:HD21	1:L:671:ILE:HG22	2.03	0.41
1:L:692:ILE:HD13	1:L:699:LEU:HD11	2.03	0.41
1:A:15:GLN:O	1:A:19:ASP:OD2	2.38	0.41
1:A:784:TRP:HB3	1:A:803:LEU:HD11	2.00	0.41
1:B:649:VAL:O	1:B:649:VAL:HG13	2.20	0.41
1:B:784:TRP:CE3	1:B:806:TRP:CD1	3.08	0.41
1:C:804:VAL:HA	1:C:826:ASN:OD1	2.20	0.41
1:D:117:LYS:O	1:D:121:ILE:HG22	2.20	0.41
1:D:680:VAL:O	1:D:684:THR:HG23	2.20	0.41
1:E:687:LEU:HD23	1:E:689:LYS:H	1.85	0.41
1:E:751:LEU:HG	1:E:776:GLU:HB3	2.01	0.41
1:H:254:LEU:HD23	1:H:254:LEU:HA	1.96	0.41
1:H:700:LEU:HB2	1:H:733:LEU:HD22	2.00	0.41
1:I:334:GLU:OE1	1:I:334:GLU:N	2.38	0.41
1:J:104:VAL:HG13	1:J:105:LYS:N	2.34	0.41
1:J:664:SER:O	1:J:665:LEU:C	2.58	0.41
1:J:784:TRP:CE3	1:J:806:TRP:CD1	3.08	0.41
1:K:692:ILE:HG22	1:K:693:ARG:N	2.35	0.41
1:L:463:VAL:HG11	1:L:466:ARG:CZ	2.50	0.41
1:A:209:ARG:O	1:A:210:ILE:HD13	2.21	0.41
1:B:214:VAL:O	1:B:214:VAL:HG12	2.19	0.41
1:B:421:ILE:HD12	1:B:475:CYS:O	2.21	0.41
1:C:174:ASN:ND2	1:C:284:ASN:O	2.53	0.41
1:D:63:VAL:HA	1:D:66:ILE:HD12	2.02	0.41
1:D:429:LEU:CD2	1:D:591:TYR:CE2	3.04	0.41
1:D:513:LEU:HB3	1:D:535:ALA:HB2	2.03	0.41
1:E:409:PHE:CD2	1:E:485:CYS:SG	3.13	0.41
1:E:816:LEU:HD21	1:E:818:HIS:O	2.21	0.41
1:F:210:ILE:HB	1:F:262:VAL:HG12	2.02	0.41
1:H:198:LYS:HE3	1:H:198:LYS:CA	2.42	0.41
1:H:214:VAL:O	1:H:266:ASP:O	2.38	0.41
1:H:467:THR:HG22	1:H:468:SER:N	2.35	0.41
1:I:214:VAL:O	1:I:266:ASP:O	2.38	0.41
1:I:714:LEU:CD1	1:I:717:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:806:TRP:CH2	1:I:834:LEU:HD11	2.55	0.41
1:J:22:GLU:OE1	1:J:22:GLU:N	2.46	0.41
1:K:103:ARG:C	1:K:103:ARG:CD	2.89	0.41
1:K:231:PHE:CE2	1:K:253:PHE:HB3	2.56	0.41
1:K:586:LEU:O	1:K:609:LEU:HD23	2.21	0.41
1:K:660:LEU:HB2	1:K:683:ARG:HE	1.85	0.41
1:L:735:LEU:HD13	1:L:763:LEU:HD21	2.02	0.41
1:L:845:LEU:CD1	1:L:848:SER:CB	2.82	0.41
1:A:82:ILE:O	1:A:86:LEU:CD2	2.60	0.41
1:A:103:ARG:HD2	1:A:106:GLU:HB3	2.02	0.41
1:A:154:ASP:N	1:A:154:ASP:OD1	2.53	0.41
1:A:214:VAL:O	1:A:266:ASP:O	2.38	0.41
1:A:590:ARG:HA	1:A:612:ILE:HA	2.02	0.41
1:B:401:LEU:CD2	1:B:406:LYS:HA	2.51	0.41
1:B:458:ARG:O	1:B:459:ASN:HB2	2.20	0.41
1:C:625:ASP:OD2	1:C:627:GLN:NE2	2.50	0.41
1:D:107:VAL:O	1:D:111:ILE:HG13	2.21	0.41
1:D:149:VAL:HG22	1:D:150:VAL:N	2.35	0.41
1:D:439:LYS:O	1:D:439:LYS:CG	2.68	0.41
1:E:480:MET:O	1:E:483:GLU:HG3	2.20	0.41
1:E:630:ILE:CG2	1:E:633:MET:HE3	2.50	0.41
1:F:154:ASP:OD1	1:F:154:ASP:C	2.58	0.41
1:F:525:VAL:HG13	1:F:526:LEU:HD22	2.03	0.41
1:F:741:PHE:N	1:F:741:PHE:CD1	2.88	0.41
1:H:197:TYR:HD2	1:H:198:LYS:HD2	1.85	0.41
1:J:105:LYS:HG3	1:J:106:GLU:H	1.86	0.41
1:K:73:ALA:O	1:K:77:ILE:HG12	2.21	0.41
1:L:463:VAL:HG11	1:L:466:ARG:NH1	2.35	0.41
1:A:400:ARG:N	1:A:400:ARG:HD2	2.35	0.41
1:A:862:LYS:O	1:A:866:GLN:HG3	2.21	0.41
1:A:881:PHE:HB2	1:A:882:PRO:HD3	2.02	0.41
1:B:113:ALA:HB1	1:B:117:LYS:HZ1	1.85	0.41
1:B:345:LYS:HZ3	1:B:378:SER:CB	2.34	0.41
1:C:174:ASN:ND2	1:C:284:ASN:HB3	2.35	0.41
1:C:260:TYR:CD1	1:C:260:TYR:C	2.94	0.41
1:C:463:VAL:HG11	1:C:466:ARG:CZ	2.51	0.41
1:C:499:ILE:HB	1:C:521:ILE:CD1	2.51	0.41
1:E:501:LEU:O	1:E:501:LEU:HD12	2.20	0.41
1:F:660:LEU:HD12	1:F:683:ARG:HH21	1.85	0.41
1:H:190:THR:HG22	3:H:902:ADP:PB	2.60	0.41
1:H:238:TYR:O	1:H:246:LEU:HD21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:SER:O	1:I:34:LEU:C	2.59	0.41
1:I:755:LEU:HB2	1:I:779:PHE:CD1	2.55	0.41
1:I:797:TRP:CE2	1:I:820:VAL:HG11	2.55	0.41
1:J:363:LYS:HE3	1:J:400:ARG:HE	1.85	0.41
1:J:845:LEU:HD11	1:J:848:SER:OG	2.20	0.41
1:K:735:LEU:HD13	1:K:763:LEU:HD21	2.03	0.41
1:L:223:LEU:HD23	1:L:223:LEU:C	2.41	0.41
1:B:92:VAL:HG12	1:B:94:ARG:H	1.86	0.41
1:B:155:VAL:HG13	3:B:902:ADP:C6	2.55	0.41
1:D:115:ARG:NE	1:D:116:ASN:OD1	2.41	0.41
1:D:373:VAL:O	1:D:377:VAL:HG23	2.21	0.41
1:D:862:LYS:HD3	1:D:862:LYS:O	2.20	0.41
1:E:149:VAL:HG12	1:E:150:VAL:N	2.35	0.41
1:E:684:THR:OG1	1:E:687:LEU:HD12	2.21	0.41
1:E:795:VAL:HG22	1:E:818:HIS:HB3	2.03	0.41
1:G:255:GLY:O	1:G:285:LYS:NZ	2.53	0.41
1:H:398:TYR:CE1	1:H:406:LYS:HG2	2.56	0.41
1:H:829:GLU:OE1	1:H:829:GLU:CA	2.69	0.41
1:H:854:ILE:O	1:H:858:GLN:HG2	2.20	0.41
1:I:309:LEU:HD12	1:I:309:LEU:HA	1.97	0.41
1:I:354:VAL:O	1:I:459:ASN:ND2	2.50	0.41
1:I:610:TRP:CZ3	1:I:611:ASN:OD1	2.74	0.41
1:J:157:GLY:O	1:J:310:LYS:NZ	2.40	0.41
1:J:214:VAL:O	1:J:214:VAL:HG12	2.20	0.41
1:J:610:TRP:CD1	1:J:611:ASN:N	2.89	0.41
1:K:207:PHE:CD1	1:K:883:PRO:HD2	2.56	0.41
1:K:223:LEU:HD23	1:K:227:ILE:HD12	2.03	0.41
1:A:97:ASP:O	1:A:101:TYR:CB	2.68	0.41
1:A:295:ASP:OD1	1:A:296:SER:N	2.53	0.41
1:B:170:LEU:HD21	1:B:205:GLU:HG2	2.03	0.41
1:B:598:SER:O	1:B:598:SER:OG	2.38	0.41
1:B:709:LYS:HG3	1:B:710:ASN:N	2.36	0.41
1:C:433:GLU:CD	1:C:568:VAL:HG21	2.41	0.41
1:D:64:LYS:HD2	1:D:65:LYS:HB3	2.02	0.41
1:D:83:GLU:OE1	1:D:104:VAL:CG1	2.69	0.41
1:D:83:GLU:OE1	1:D:104:VAL:HG12	2.21	0.41
1:D:199:HIS:HB3	1:D:202:ILE:HG12	2.02	0.41
1:F:83:GLU:OE2	1:F:103:ARG:HD2	2.19	0.41
1:F:602:LEU:HD12	1:F:602:LEU:HA	1.97	0.41
1:G:82:ILE:O	1:G:86:LEU:HD23	2.21	0.41
1:G:161:GLU:O	1:G:165:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:735:LEU:HD13	1:G:763:LEU:HD21	2.02	0.41
1:H:670:THR:OG1	1:H:670:THR:O	2.39	0.41
1:H:753:THR:OG1	1:H:778:GLY:O	2.34	0.41
1:I:254:LEU:HD11	1:I:260:TYR:CG	2.56	0.41
1:I:724:ASN:HB3	1:I:752:ASP:O	2.21	0.41
1:J:414:ALA:O	1:J:522:HIS:CE1	2.73	0.41
1:K:87:HIS:CE1	1:K:104:VAL:HG21	2.55	0.41
1:K:105:LYS:O	1:K:108:ALA:HB3	2.20	0.41
1:A:403:TYR:HA	1:A:406:LYS:HD2	2.03	0.41
1:A:751:LEU:HA	1:A:775:LYS:O	2.21	0.41
1:A:845:LEU:HB3	1:A:880:ILE:HG22	2.03	0.41
1:C:525:VAL:HG21	1:C:541:PHE:HZ	1.85	0.41
1:D:58:VAL:O	1:D:62:LEU:HG	2.21	0.41
1:D:160:GLU:O	1:D:163:ASP:OD1	2.39	0.41
1:D:853:ALA:HB2	1:D:885:LEU:HB3	2.03	0.41
1:E:163:ASP:OD1	1:E:164:ILE:N	2.54	0.41
1:E:174:ASN:HA	1:E:285:LYS:CA	2.51	0.41
1:E:878:LEU:HD12	1:E:879:SER:N	2.36	0.41
1:F:660:LEU:HB2	1:F:683:ARG:HE	1.86	0.41
1:F:785:GLU:O	1:F:785:GLU:HG2	2.21	0.41
1:G:149:VAL:HG22	1:G:150:VAL:N	2.36	0.41
1:G:169:LEU:HD11	1:G:206:PHE:HE2	1.85	0.41
1:G:320:LEU:HD13	3:G:902:ADP:C2	2.56	0.41
1:G:622:ARG:HA	1:G:622:ARG:CZ	2.50	0.41
1:H:350:PRO:HB2	3:H:902:ADP:HI'	2.03	0.41
1:H:718:GLU:HG3	1:H:718:GLU:O	2.21	0.41
1:J:64:LYS:HD2	1:J:65:LYS:HB3	2.03	0.41
1:J:87:HIS:HD2	1:J:106:GLU:OE2	2.04	0.41
1:J:117:LYS:O	1:J:121:ILE:HG12	2.21	0.41
1:J:241:MET:HE3	1:J:245:ASP:OD1	2.20	0.41
1:J:350:PRO:HB3	3:J:902:ADP:C4	2.56	0.41
1:J:463:VAL:HG21	1:J:472:ILE:CD1	2.51	0.41
1:K:66:ILE:O	1:K:70:VAL:HG13	2.21	0.41
1:K:172:GLU:O	1:K:288:ARG:NH2	2.53	0.41
1:K:194:ASN:O	1:K:198:LYS:HG2	2.20	0.41
1:K:220:ARG:HD3	1:K:275:ARG:HE	1.85	0.41
1:K:687:LEU:HD23	1:K:689:LYS:H	1.86	0.41
1:L:155:VAL:HG12	1:L:158:PHE:HD2	1.84	0.41
1:A:27:VAL:O	1:A:27:VAL:CG2	2.68	0.41
1:C:480:MET:O	1:C:483:GLU:HG3	2.21	0.41
1:C:660:LEU:H	1:C:660:LEU:CD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASN:O	1:D:175:HIS:HB2	2.21	0.41
1:E:499:ILE:HG13	1:E:519:LEU:HD22	2.03	0.41
1:F:352:ALA:HA	1:F:393:LEU:HD23	2.03	0.41
1:F:376:SER:HB3	1:F:396:MET:SD	2.61	0.41
1:F:550:GLU:OE1	1:F:550:GLU:N	2.54	0.41
1:F:753:THR:OG1	1:F:778:GLY:O	2.37	0.41
1:G:356:ILE:HG12	1:G:393:LEU:HD22	2.03	0.41
1:G:696:ILE:O	1:G:696:ILE:HG22	2.21	0.41
1:G:865:ASN:OD1	1:G:865:ASN:O	2.39	0.41
1:H:80:PHE:HD2	1:H:111:ILE:CD1	2.33	0.41
1:H:612:ILE:HD12	1:H:615:ILE:HD11	2.01	0.41
1:I:776:GLU:OE1	1:I:776:GLU:O	2.38	0.41
1:J:207:PHE:HD2	1:J:883:PRO:HD2	1.86	0.41
1:K:354:VAL:CG1	1:K:459:ASN:HB3	2.51	0.41
1:L:174:ASN:O	1:L:174:ASN:OD1	2.39	0.41
1:L:401:LEU:HG	1:L:405:LEU:CB	2.51	0.41
1:A:584:TYR:CD1	1:A:584:TYR:N	2.87	0.40
1:A:755:LEU:HB2	1:A:779:PHE:CD1	2.57	0.40
1:B:483:GLU:HG3	1:B:484:PHE:H	1.86	0.40
1:C:42:ASN:HA	1:C:45:LEU:HD12	2.03	0.40
1:C:180:PRO:HA	1:C:291:LEU:HG	2.02	0.40
1:C:811:ASP:OD1	1:C:812:ASP:N	2.54	0.40
1:D:34:LEU:O	1:D:38:LEU:HG	2.21	0.40
1:D:535:ALA:O	1:D:562:GLY:O	2.39	0.40
1:E:549:ILE:HG22	1:E:550:GLU:O	2.21	0.40
1:E:602:LEU:HD12	1:E:602:LEU:HA	1.97	0.40
1:E:609:LEU:HD12	1:E:609:LEU:N	2.36	0.40
1:F:166:ILE:HG23	1:F:202:ILE:HD11	2.02	0.40
1:F:642:ASN:OD1	1:F:642:ASN:C	2.60	0.40
1:G:295:ASP:HB3	1:G:298:VAL:HG22	2.03	0.40
1:G:865:ASN:OD1	1:G:865:ASN:C	2.59	0.40
1:H:98:LEU:HB2	1:H:99:PRO:HD3	2.03	0.40
1:I:244:GLU:OE2	1:I:278:ILE:HD12	2.21	0.40
1:I:325:VAL:HG23	1:I:361:ILE:CD1	2.51	0.40
1:I:463:VAL:O	1:I:463:VAL:HG13	2.20	0.40
1:I:467:THR:HG22	1:I:468:SER:H	1.86	0.40
1:J:424:TRP:CZ3	1:J:640:HIS:CE1	3.08	0.40
1:J:502:GLY:O	1:J:505:GLN:N	2.49	0.40
1:J:558:THR:HG23	1:J:559:ILE:N	2.35	0.40
1:K:83:GLU:OE2	1:K:103:ARG:CD	2.67	0.40
1:K:405:LEU:HD13	1:K:405:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:238:TYR:HB3	1:L:246:LEU:HD21	2.04	0.40
1:L:355:VAL:HG22	1:L:397:SER:OG	2.21	0.40
1:B:357:ALA:O	1:B:361:ILE:HG22	2.21	0.40
1:C:115:ARG:HA	1:C:118:VAL:HG22	2.03	0.40
1:C:177:GLU:H	1:C:288:ARG:HH21	1.68	0.40
1:C:480:MET:HA	1:C:483:GLU:HG2	2.03	0.40
1:C:749:THR:HA	1:C:773:LYS:O	2.21	0.40
1:D:398:TYR:CE1	1:D:406:LYS:HG2	2.56	0.40
1:E:401:LEU:HD22	1:E:406:LYS:HA	2.03	0.40
1:F:38:LEU:HD21	1:F:70:VAL:HG22	2.03	0.40
1:F:149:VAL:HG22	1:F:150:VAL:H	1.85	0.40
1:F:782:GLU:N	1:F:782:GLU:CD	2.75	0.40
1:H:401:LEU:HB3	1:H:406:LYS:CG	2.51	0.40
1:H:755:LEU:HD12	1:H:779:PHE:HE1	1.85	0.40
1:J:174:ASN:ND2	1:J:284:ASN:O	2.54	0.40
1:J:229:SER:O	1:J:233:ARG:NH2	2.54	0.40
1:J:714:LEU:HD12	1:J:717:LEU:CD1	2.49	0.40
1:K:794:LEU:HB3	1:K:817:LYS:HG3	2.03	0.40
1:L:192:LEU:CD1	1:L:196:ILE:HD11	2.51	0.40
1:L:717:LEU:HD23	1:L:718:GLU:N	2.36	0.40
1:A:169:LEU:CD1	1:A:170:LEU:HB2	2.51	0.40
1:A:746:ARG:HG2	1:A:746:ARG:O	2.21	0.40
1:A:784:TRP:CB	1:A:803:LEU:HD11	2.51	0.40
1:C:212:VAL:HB	1:C:264:LEU:HD23	2.04	0.40
1:D:209:ARG:HA	1:D:261:LEU:O	2.20	0.40
1:D:521:ILE:HG21	1:D:525:VAL:HB	2.04	0.40
1:D:735:LEU:CD1	1:D:763:LEU:HD21	2.51	0.40
1:E:763:LEU:HD23	1:E:763:LEU:N	2.36	0.40
1:F:818:HIS:HA	1:F:842:VAL:O	2.21	0.40
1:G:83:GLU:O	1:G:83:GLU:OE2	2.39	0.40
1:H:390:CYS:O	1:H:394:VAL:HG23	2.20	0.40
1:H:700:LEU:CB	1:H:733:LEU:HD22	2.51	0.40
1:I:244:GLU:HG2	1:L:511:ARG:HH12	1.86	0.40
1:I:401:LEU:HD21	1:I:405:LEU:HB3	2.03	0.40
1:J:15:GLN:HG3	1:J:19:ASP:OD2	2.21	0.40
1:K:158:PHE:CD2	3:K:902:ADP:N1	2.89	0.40
1:K:401:LEU:O	1:K:406:LYS:HE3	2.22	0.40
1:K:435:PHE:N	1:K:435:PHE:CD1	2.85	0.40
1:K:597:ASP:OD1	1:K:597:ASP:N	2.55	0.40
1:L:341:SER:OG	1:L:374:ASP:OD2	2.33	0.40
1:L:461:VAL:CG1	1:L:475:CYS:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:782:GLU:O	1:L:804:VAL:N	2.47	0.40
1:L:795:VAL:HG22	1:L:818:HIS:HB3	2.02	0.40
1:A:345:LYS:NZ	1:A:374:ASP:OD1	2.52	0.40
1:A:609:LEU:N	1:A:609:LEU:HD12	2.36	0.40
1:A:688:LYS:O	1:A:688:LYS:CG	2.69	0.40
1:C:40:ASP:OD1	1:C:41:PHE:N	2.54	0.40
1:C:320:LEU:HD21	3:C:902:ADP:N1	2.35	0.40
1:C:410:LEU:HD12	1:C:485:CYS:SG	2.61	0.40
1:C:575:ASN:OD1	1:C:576:PHE:N	2.54	0.40
1:C:721:LYS:HD2	1:C:723:ILE:HD11	2.03	0.40
1:D:41:PHE:CD1	1:D:41:PHE:N	2.89	0.40
1:D:467:THR:N	1:D:471:GLN:O	2.43	0.40
1:D:544:PHE:CE1	1:D:570:ASP:OD2	2.74	0.40
1:E:173:SER:HA	1:E:286:PRO:HB3	2.03	0.40
1:E:456:ILE:HD11	1:E:472:ILE:HD13	2.03	0.40
1:F:8:PHE:HD1	1:F:8:PHE:O	2.04	0.40
1:F:695:LYS:CG	1:F:698:VAL:HG23	2.52	0.40
1:H:273:TRP:O	1:H:273:TRP:CE3	2.74	0.40
1:I:19:ASP:OD1	1:I:19:ASP:C	2.60	0.40
1:J:107:VAL:O	1:J:107:VAL:CG1	2.69	0.40
1:J:147:PRO:HA	1:J:148:PRO:HD3	1.87	0.40
1:J:344:LYS:O	1:J:344:LYS:HD2	2.22	0.40
1:J:590:ARG:HA	1:J:612:ILE:HA	2.02	0.40
1:K:211:TRP:CZ3	1:K:263:VAL:HG11	2.56	0.40
1:K:354:VAL:HG21	3:K:902:ADP:H8	1.86	0.40
1:K:639:LEU:O	1:K:639:LEU:HD23	2.21	0.40
1:K:880:ILE:O	1:K:880:ILE:HG13	2.22	0.40
1:L:74:GLU:O	1:L:77:ILE:HG22	2.21	0.40
1:L:163:ASP:OD1	1:L:163:ASP:C	2.60	0.40
1:L:473:LYS:HG2	1:L:474:THR:HG22	2.03	0.40
1:L:816:LEU:HD22	1:L:840:PHE:CE1	2.56	0.40
1:A:223:LEU:O	1:A:227:ILE:HG13	2.21	0.40
1:A:345:LYS:HZ3	1:A:378:SER:HB3	1.86	0.40
1:A:647:LEU:HD12	1:A:671:ILE:HD12	2.01	0.40
1:A:806:TRP:CE3	1:A:831:PRO:HD2	2.57	0.40
1:B:74:GLU:O	1:B:78:ASP:OD1	2.39	0.40
1:C:267:VAL:O	1:C:293:THR:OG1	2.25	0.40
1:C:596:SER:HB2	1:C:599:ILE:HG22	2.03	0.40
1:F:428:ARG:NH1	1:F:640:HIS:HD2	2.20	0.40
1:G:316:GLU:HA	1:G:319:ILE:HG22	2.04	0.40
1:G:513:LEU:HB3	1:G:535:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:755:LEU:HB3	1:G:779:PHE:CE2	2.56	0.40
1:H:777:ASN:N	1:H:800:ARG:O	2.54	0.40
1:I:325:VAL:HG13	1:I:326:PHE:CD2	2.57	0.40
1:I:463:VAL:HG21	1:I:472:ILE:HD12	2.02	0.40
1:I:838:ARG:HA	1:I:838:ARG:NE	2.37	0.40
1:J:65:LYS:O	1:J:69:VAL:HG23	2.22	0.40
1:K:259:LYS:CE	1:K:286:PRO:HD2	2.51	0.40
1:K:393:LEU:HD12	1:K:396:MET:HE2	2.04	0.40
1:K:531:THR:O	1:K:531:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	883/885 (100%)	813 (92%)	70 (8%)	0	100	100
1	B	883/885 (100%)	820 (93%)	63 (7%)	0	100	100
1	C	883/885 (100%)	843 (96%)	39 (4%)	1 (0%)	48	79
1	D	883/885 (100%)	835 (95%)	48 (5%)	0	100	100
1	E	883/885 (100%)	806 (91%)	74 (8%)	3 (0%)	37	67
1	F	883/885 (100%)	834 (94%)	49 (6%)	0	100	100
1	G	883/885 (100%)	839 (95%)	44 (5%)	0	100	100
1	H	883/885 (100%)	818 (93%)	64 (7%)	1 (0%)	48	79
1	I	883/885 (100%)	824 (93%)	59 (7%)	0	100	100
1	J	883/885 (100%)	804 (91%)	78 (9%)	1 (0%)	48	79
1	K	883/885 (100%)	821 (93%)	61 (7%)	1 (0%)	48	79
1	L	883/885 (100%)	836 (95%)	47 (5%)	0	100	100
All	All	10596/10620 (100%)	9893 (93%)	696 (7%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	408	CYS
1	E	409	PHE
1	H	65	LYS
1	K	147	PRO
1	J	107	VAL
1	C	148	PRO
1	E	121	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	797/797 (100%)	782 (98%)	15 (2%)	52	73
1	B	797/797 (100%)	779 (98%)	18 (2%)	45	68
1	C	797/797 (100%)	773 (97%)	24 (3%)	36	63
1	D	797/797 (100%)	783 (98%)	14 (2%)	54	74
1	E	797/797 (100%)	767 (96%)	30 (4%)	28	57
1	F	797/797 (100%)	780 (98%)	17 (2%)	48	71
1	G	797/797 (100%)	781 (98%)	16 (2%)	50	72
1	H	797/797 (100%)	780 (98%)	17 (2%)	48	71
1	I	797/797 (100%)	783 (98%)	14 (2%)	54	74
1	J	797/797 (100%)	768 (96%)	29 (4%)	30	59
1	K	797/797 (100%)	778 (98%)	19 (2%)	44	67
1	L	797/797 (100%)	782 (98%)	15 (2%)	52	73
All	All	9564/9564 (100%)	9336 (98%)	228 (2%)	45	67

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	115	ARG

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Mol	Chain	Res	Type
1	A	153	ASP
1	A	169	LEU
1	A	176	LEU
1	A	184	MET
1	A	207	PHE
1	A	239	HIS
1	A	242	CYS
1	A	315	ASP
1	A	643	SER
1	A	695	LYS
1	A	758	LYS
1	A	811	ASP
1	A	836	ASP
1	B	15	GLN
1	B	64	LYS
1	B	78	ASP
1	B	123	GLN
1	B	125	ASP
1	B	132	LEU
1	B	159	ASP
1	B	204	TYR
1	B	217	SER
1	B	390	CYS
1	B	438	TYR
1	B	483	GLU
1	B	487	GLN
1	B	579	PHE
1	B	591	TYR
1	B	630	ILE
1	B	702	ASN
1	B	776	GLU
1	C	3	ASN
1	C	130	GLN
1	C	146	LYS
1	C	152	GLU
1	C	159	ASP
1	C	169	LEU
1	C	177	GLU
1	C	189	LYS
1	C	206	PHE
1	C	208	THR
1	C	253	PHE

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Mol	Chain	Res	Type
1	C	310	LYS
1	C	398	TYR
1	C	469	ASP
1	C	483	GLU
1	C	501	LEU
1	C	551	MET
1	C	622	ARG
1	C	664	SER
1	C	719	ASN
1	C	805	SER
1	C	857	ARG
1	C	866	GLN
1	C	877	LYS
1	D	41	PHE
1	D	64	LYS
1	D	83	GLU
1	D	125	ASP
1	D	158	PHE
1	D	177	GLU
1	D	242	CYS
1	D	310	LYS
1	D	378	SER
1	D	403	TYR
1	D	413	SER
1	D	441	HIS
1	D	606	MET
1	D	701	ASP
1	E	3	ASN
1	E	15	GLN
1	E	62	LEU
1	E	64	LYS
1	E	78	ASP
1	E	115	ARG
1	E	120	GLU
1	E	123	GLN
1	E	158	PHE
1	E	159	ASP
1	E	204	TYR
1	E	217	SER
1	E	242	CYS
1	E	252	GLU
1	E	310	LYS

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Mol	Chain	Res	Type
1	E	315	ASP
1	E	327	HIS
1	E	390	CYS
1	E	409	PHE
1	E	412	CYS
1	E	425	LYS
1	E	438	TYR
1	E	487	GLN
1	E	591	TYR
1	E	597	ASP
1	E	703	LYS
1	E	719	ASN
1	E	753	THR
1	E	877	LYS
1	E	881	PHE
1	F	8	PHE
1	F	59	LEU
1	F	115	ARG
1	F	159	ASP
1	F	215	SER
1	F	259	LYS
1	F	310	LYS
1	F	439	LYS
1	F	486	ARG
1	F	494	ASN
1	F	504	GLU
1	F	591	TYR
1	F	640	HIS
1	F	736	PRO
1	F	791	CYS
1	F	843	MET
1	F	881	PHE
1	G	78	ASP
1	G	130	GLN
1	G	158	PHE
1	G	159	ASP
1	G	167	ASN
1	G	169	LEU
1	G	177	GLU
1	G	215	SER
1	G	310	LYS
1	G	378	SER

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Mol	Chain	Res	Type
1	G	441	HIS
1	G	469	ASP
1	G	686	ASN
1	G	721	LYS
1	G	844	MET
1	G	877	LYS
1	H	1	MET
1	H	78	ASP
1	H	80	PHE
1	H	102	LYS
1	H	115	ARG
1	H	158	PHE
1	H	216	GLN
1	H	242	CYS
1	H	283	ASN
1	H	294	ARG
1	H	408	CYS
1	H	412	CYS
1	H	450	ASP
1	H	545	SER
1	H	597	ASP
1	H	622	ARG
1	H	881	PHE
1	I	64	LYS
1	I	174	ASN
1	I	221	ARG
1	I	242	CYS
1	I	404	ASP
1	I	475	CYS
1	I	510	LYS
1	I	545	SER
1	I	591	TYR
1	I	597	ASP
1	I	734	ARG
1	I	800	ARG
1	I	811	ASP
1	I	838	ARG
1	J	3	ASN
1	J	103	ARG
1	J	107	VAL
1	J	123	GLN
1	J	125	ASP

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Mol	Chain	Res	Type
1	J	158	PHE
1	J	159	ASP
1	J	177	GLU
1	J	204	TYR
1	J	217	SER
1	J	220	ARG
1	J	271	GLU
1	J	277	LYS
1	J	287	ASN
1	J	307	HIS
1	J	310	LYS
1	J	315	ASP
1	J	408	CYS
1	J	438	TYR
1	J	441	HIS
1	J	501	LEU
1	J	563	PHE
1	J	564	PRO
1	J	591	TYR
1	J	606	MET
1	J	686	ASN
1	J	701	ASP
1	J	836	ASP
1	J	844	MET
1	K	64	LYS
1	K	97	ASP
1	K	110	GLU
1	K	146	LYS
1	K	159	ASP
1	K	169	LEU
1	K	177	GLU
1	K	310	LYS
1	K	385	ASP
1	K	401	LEU
1	K	449	GLU
1	K	486	ARG
1	K	487	GLN
1	K	501	LEU
1	K	591	TYR
1	K	597	ASP
1	K	640	HIS
1	K	643	SER

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Mol	Chain	Res	Type
1	K	776	GLU
1	L	41	PHE
1	L	101	TYR
1	L	115	ARG
1	L	159	ASP
1	L	177	GLU
1	L	221	ARG
1	L	242	CYS
1	L	301	GLN
1	L	310	LYS
1	L	327	HIS
1	L	400	ARG
1	L	437	GLN
1	L	441	HIS
1	L	474	THR
1	L	505	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	HIS
1	A	777	ASN
1	B	380	HIS
1	B	522	HIS
1	B	686	ASN
1	C	451	ASN
1	D	100	HIS
1	D	234	ASN
1	E	71	ASN
1	E	420	GLN
1	E	522	HIS
1	E	588	HIS
1	F	478	HIS
1	F	640	HIS
1	F	841	GLN
1	F	868	GLN
1	G	39	ASN
1	G	174	ASN
1	G	175	HIS
1	G	640	HIS
1	H	478	HIS
1	I	39	ASN

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Mol	Chain	Res	Type
1	I	777	ASN
1	I	818	HIS
1	J	818	HIS
1	J	866	GLN
1	J	868	GLN
1	K	327	HIS
1	K	453	ASN
1	K	478	HIS
1	K	640	HIS
1	L	437	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IHP	H	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.73	2 (3%)
2	IHP	B	901	-	36,36,36	0.76	0	54,60,60	0.60	0
3	ADP	G	902	-	24,29,29	0.69	0	29,45,45	0.92	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	J	902	-	24,29,29	0.73	0	29,45,45	0.78	0
2	IHP	C	901	-	36,36,36	1.48	6 (16%)	54,60,60	0.57	0
3	ADP	B	902	-	24,29,29	0.72	0	29,45,45	0.78	1 (3%)
2	IHP	L	901	-	36,36,36	1.43	6 (16%)	54,60,60	0.64	1 (1%)
3	ADP	D	902	-	24,29,29	0.71	0	29,45,45	0.85	1 (3%)
3	ADP	F	902	-	24,29,29	0.70	1 (4%)	29,45,45	0.79	1 (3%)
2	IHP	K	901	-	36,36,36	1.44	6 (16%)	54,60,60	0.61	0
2	IHP	I	901	-	36,36,36	1.42	6 (16%)	54,60,60	0.59	0
3	ADP	H	902	-	24,29,29	0.74	0	29,45,45	0.82	1 (3%)
2	IHP	A	901	-	36,36,36	0.74	0	54,60,60	0.63	0
3	ADP	I	902	-	24,29,29	0.73	1 (4%)	29,45,45	0.78	1 (3%)
3	ADP	C	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
2	IHP	E	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.65	1 (1%)
3	ADP	L	902	-	24,29,29	0.70	0	29,45,45	0.88	0
2	IHP	J	901	-	36,36,36	0.74	0	54,60,60	0.54	0
3	ADP	K	902	-	24,29,29	0.67	0	29,45,45	0.92	2 (6%)
3	ADP	A	902	-	24,29,29	0.79	0	29,45,45	0.79	1 (3%)
2	IHP	G	901	-	36,36,36	0.75	0	54,60,60	0.61	0
2	IHP	D	901	-	36,36,36	0.76	0	54,60,60	0.56	0
2	IHP	F	901	-	36,36,36	0.73	0	54,60,60	0.56	0
3	ADP	E	902	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	H	901	-	-	16/30/54/54	0/1/1/1
2	IHP	B	901	-	-	15/30/54/54	0/1/1/1
3	ADP	G	902	-	-	7/12/32/32	0/3/3/3
3	ADP	J	902	-	-	1/12/32/32	0/3/3/3
2	IHP	C	901	-	-	7/30/54/54	0/1/1/1
3	ADP	B	902	-	-	1/12/32/32	0/3/3/3
2	IHP	L	901	-	-	14/30/54/54	0/1/1/1
3	ADP	D	902	-	-	5/12/32/32	0/3/3/3
3	ADP	F	902	-	-	9/12/32/32	0/3/3/3
2	IHP	K	901	-	-	12/30/54/54	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	I	901	-	-	7/30/54/54	0/1/1/1
3	ADP	H	902	-	-	5/12/32/32	0/3/3/3
2	IHP	A	901	-	-	11/30/54/54	0/1/1/1
3	ADP	I	902	-	-	4/12/32/32	0/3/3/3
3	ADP	C	902	-	-	5/12/32/32	0/3/3/3
2	IHP	E	901	-	-	18/30/54/54	0/1/1/1
3	ADP	L	902	-	-	5/12/32/32	0/3/3/3
2	IHP	J	901	-	-	7/30/54/54	0/1/1/1
3	ADP	K	902	-	-	4/12/32/32	0/3/3/3
3	ADP	A	902	-	-	5/12/32/32	0/3/3/3
2	IHP	G	901	-	-	13/30/54/54	0/1/1/1
2	IHP	D	901	-	-	8/30/54/54	0/1/1/1
2	IHP	F	901	-	-	8/30/54/54	0/1/1/1
3	ADP	E	902	-	-	6/12/32/32	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	IHP	P4-O14	3.41	1.65	1.59
2	H	901	IHP	P5-O15	3.28	1.65	1.59
2	K	901	IHP	P6-O16	3.27	1.65	1.59
2	C	901	IHP	P6-O16	3.23	1.65	1.59
2	C	901	IHP	P4-O14	3.20	1.65	1.59
2	H	901	IHP	P4-O14	3.19	1.65	1.59
2	C	901	IHP	P2-O12	3.17	1.65	1.59
2	K	901	IHP	P1-O11	3.15	1.65	1.59
2	C	901	IHP	P1-O11	3.14	1.65	1.59
2	C	901	IHP	P3-O13	3.14	1.65	1.59
2	L	901	IHP	P5-O15	3.14	1.65	1.59
2	K	901	IHP	P4-O14	3.14	1.65	1.59
2	I	901	IHP	P1-O11	3.11	1.65	1.59
2	C	901	IHP	P5-O15	3.10	1.65	1.59
2	L	901	IHP	P1-O11	3.10	1.65	1.59
2	E	901	IHP	P6-O16	3.10	1.65	1.59
2	H	901	IHP	P1-O11	3.08	1.65	1.59
2	L	901	IHP	P4-O14	3.04	1.65	1.59
2	I	901	IHP	P6-O16	3.04	1.65	1.59
2	E	901	IHP	P1-O11	3.03	1.65	1.59
2	E	901	IHP	P3-O13	3.03	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	901	IHP	P3-O13	3.00	1.65	1.59
2	I	901	IHP	P4-O14	2.99	1.65	1.59
2	L	901	IHP	P6-O16	2.99	1.65	1.59
2	K	901	IHP	P2-O12	2.99	1.65	1.59
2	I	901	IHP	P3-O13	2.96	1.64	1.59
2	I	901	IHP	P5-O15	2.95	1.64	1.59
2	E	901	IHP	P2-O12	2.95	1.64	1.59
2	H	901	IHP	P2-O12	2.94	1.64	1.59
2	L	901	IHP	P2-O12	2.93	1.64	1.59
2	H	901	IHP	P6-O16	2.89	1.64	1.59
2	I	901	IHP	P2-O12	2.88	1.64	1.59
2	H	901	IHP	P3-O13	2.88	1.64	1.59
2	E	901	IHP	P5-O15	2.87	1.64	1.59
2	K	901	IHP	P3-O13	2.84	1.64	1.59
2	K	901	IHP	P5-O15	2.75	1.64	1.59
3	C	902	ADP	C5-C4	2.37	1.47	1.40
3	F	902	ADP	C8-N7	-2.09	1.31	1.34
3	I	902	ADP	C8-N7	-2.02	1.31	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	ADP	N3-C2-N1	-3.61	123.03	128.68
3	C	902	ADP	PA-O3A-PB	-3.11	122.16	132.83
2	H	901	IHP	C4-C3-C2	2.69	116.31	110.41
3	C	902	ADP	C3'-C2'-C1'	2.43	104.64	100.98
3	G	902	ADP	C5-C6-N6	2.39	123.98	120.35
3	K	902	ADP	C5-C6-N6	2.38	123.97	120.35
3	K	902	ADP	C3'-C2'-C1'	2.27	104.39	100.98
3	B	902	ADP	C5-C6-N6	2.22	123.72	120.35
3	D	902	ADP	C5-C6-N6	2.18	123.67	120.35
3	A	902	ADP	C5-C6-N6	2.10	123.55	120.35
3	H	902	ADP	C5-C6-N6	2.10	123.55	120.35
3	I	902	ADP	C5-C6-N6	2.10	123.54	120.35
3	C	902	ADP	C4-C5-N7	-2.06	107.25	109.40
3	F	902	ADP	C5-C6-N6	2.04	123.44	120.35
2	L	901	IHP	C5-C6-C1	2.03	114.86	110.41
2	E	901	IHP	O14-C4-C3	2.03	113.48	108.69
2	H	901	IHP	C5-C4-C3	2.02	114.83	110.41
3	E	902	ADP	C5-C6-N6	2.02	123.42	120.35
3	G	902	ADP	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	IHP	C1-C2-O12-P2
2	A	901	IHP	C3-C2-O12-P2
2	A	901	IHP	C2-C3-O13-P3
2	A	901	IHP	C3-O13-P3-O43
2	A	901	IHP	C4-O14-P4-O24
2	B	901	IHP	C2-C1-O11-P1
2	B	901	IHP	C1-C2-O12-P2
2	B	901	IHP	C3-C2-O12-P2
2	B	901	IHP	C2-C3-O13-P3
2	B	901	IHP	C4-C3-O13-P3
2	B	901	IHP	C3-C4-O14-P4
2	B	901	IHP	C5-O15-P5-O35
2	C	901	IHP	C1-C2-O12-P2
2	C	901	IHP	C3-C2-O12-P2
2	C	901	IHP	C1-O11-P1-O31
2	C	901	IHP	C4-O14-P4-O24
2	D	901	IHP	C5-C4-O14-P4
2	D	901	IHP	C6-C5-O15-P5
2	E	901	IHP	C2-C1-O11-P1
2	E	901	IHP	C6-C1-O11-P1
2	E	901	IHP	C1-C2-O12-P2
2	E	901	IHP	C3-C2-O12-P2
2	E	901	IHP	C3-C4-O14-P4
2	E	901	IHP	C4-C5-O15-P5
2	E	901	IHP	C6-C5-O15-P5
2	E	901	IHP	C1-C6-O16-P6
2	E	901	IHP	C5-C6-O16-P6
2	E	901	IHP	C2-O12-P2-O32
2	E	901	IHP	C5-O15-P5-O35
2	F	901	IHP	C3-C2-O12-P2
2	F	901	IHP	C2-C3-O13-P3
2	G	901	IHP	C3-C2-O12-P2
2	G	901	IHP	C4-C5-O15-P5
2	G	901	IHP	C6-C5-O15-P5
2	G	901	IHP	C1-C6-O16-P6
2	G	901	IHP	C5-C6-O16-P6
2	G	901	IHP	C3-O13-P3-O43
2	G	901	IHP	C5-O15-P5-O35
2	H	901	IHP	C1-C2-O12-P2
2	H	901	IHP	C3-C2-O12-P2

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Mol	Chain	Res	Type	Atoms
2	H	901	IHP	C2-C3-O13-P3
2	H	901	IHP	C4-C3-O13-P3
2	H	901	IHP	C4-O14-P4-O24
2	H	901	IHP	C6-O16-P6-O26
2	I	901	IHP	C2-C3-O13-P3
2	J	901	IHP	C4-C3-O13-P3
2	J	901	IHP	C3-C4-O14-P4
2	J	901	IHP	C5-C4-O14-P4
2	J	901	IHP	C5-O15-P5-O25
2	K	901	IHP	C1-C2-O12-P2
2	K	901	IHP	C3-C2-O12-P2
2	K	901	IHP	C4-C5-O15-P5
2	K	901	IHP	C6-C5-O15-P5
2	K	901	IHP	C5-C6-O16-P6
2	K	901	IHP	C1-O11-P1-O21
2	K	901	IHP	C4-O14-P4-O24
2	L	901	IHP	C1-C2-O12-P2
2	L	901	IHP	C3-C2-O12-P2
2	L	901	IHP	C2-C3-O13-P3
2	L	901	IHP	C4-C3-O13-P3
2	L	901	IHP	C3-C4-O14-P4
2	L	901	IHP	C5-C4-O14-P4
2	L	901	IHP	C3-O13-P3-O23
2	L	901	IHP	C5-O15-P5-O25
3	A	902	ADP	C5'-O5'-PA-O2A
3	B	902	ADP	C4'-C5'-O5'-PA
3	C	902	ADP	C5'-O5'-PA-O1A
3	D	902	ADP	C5'-O5'-PA-O2A
3	E	902	ADP	C5'-O5'-PA-O1A
3	E	902	ADP	C4'-C5'-O5'-PA
3	E	902	ADP	O4'-C4'-C5'-O5'
3	F	902	ADP	C5'-O5'-PA-O1A
3	F	902	ADP	C5'-O5'-PA-O2A
3	F	902	ADP	C4'-C5'-O5'-PA
3	F	902	ADP	C3'-C4'-C5'-O5'
3	G	902	ADP	C5'-O5'-PA-O3A
3	G	902	ADP	C4'-C5'-O5'-PA
3	G	902	ADP	C3'-C4'-C5'-O5'
3	H	902	ADP	C5'-O5'-PA-O3A
3	H	902	ADP	C4'-C5'-O5'-PA
3	I	902	ADP	C5'-O5'-PA-O1A
3	I	902	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	K	902	ADP	C4'-C5'-O5'-PA
3	K	902	ADP	C3'-C4'-C5'-O5'
3	F	902	ADP	O4'-C4'-C5'-O5'
3	G	902	ADP	O4'-C4'-C5'-O5'
3	L	902	ADP	O4'-C4'-C5'-O5'
3	E	902	ADP	C3'-C4'-C5'-O5'
3	J	902	ADP	O4'-C4'-C5'-O5'
3	K	902	ADP	O4'-C4'-C5'-O5'
2	A	901	IHP	C5-C4-O14-P4
2	B	901	IHP	C5-C4-O14-P4
2	H	901	IHP	C2-C1-O11-P1
2	H	901	IHP	C5-C4-O14-P4
3	F	902	ADP	PA-O3A-PB-O1B
2	A	901	IHP	C3-C4-O14-P4
2	D	901	IHP	C5-C6-O16-P6
2	E	901	IHP	C2-C3-O13-P3
2	E	901	IHP	C4-C3-O13-P3
2	F	901	IHP	C1-C2-O12-P2
2	H	901	IHP	C5-C6-O16-P6
3	G	902	ADP	PB-O3A-PA-O1A
3	A	902	ADP	C4'-C5'-O5'-PA
3	D	902	ADP	C4'-C5'-O5'-PA
3	A	902	ADP	PB-O3A-PA-O5'
3	G	902	ADP	PB-O3A-PA-O5'
3	L	902	ADP	PB-O3A-PA-O5'
2	E	901	IHP	C5-O15-P5-O25
2	G	901	IHP	C5-O15-P5-O25
2	L	901	IHP	C4-O14-P4-O24
3	C	902	ADP	PA-O3A-PB-O3B
3	F	902	ADP	PA-O3A-PB-O3B
2	A	901	IHP	C4-O14-P4-O34
2	B	901	IHP	C4-C5-O15-P5
2	B	901	IHP	C6-C5-O15-P5
2	B	901	IHP	C3-O13-P3-O33
2	B	901	IHP	C4-O14-P4-O34
2	C	901	IHP	C3-O13-P3-O33
2	C	901	IHP	C5-O15-P5-O45
2	D	901	IHP	C1-C6-O16-P6
2	D	901	IHP	C4-O14-P4-O34
2	F	901	IHP	C3-C4-O14-P4
2	F	901	IHP	C5-C4-O14-P4
2	F	901	IHP	C4-O14-P4-O34

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Mol	Chain	Res	Type	Atoms
2	F	901	IHP	C5-O15-P5-O45
2	G	901	IHP	C2-O12-P2-O32
2	H	901	IHP	C6-C1-O11-P1
2	H	901	IHP	C3-C4-O14-P4
2	H	901	IHP	C1-C6-O16-P6
2	H	901	IHP	C6-O16-P6-O36
2	I	901	IHP	C1-C2-O12-P2
2	K	901	IHP	C2-O12-P2-O32
2	L	901	IHP	C3-O13-P3-O43
3	C	902	ADP	C5'-O5'-PA-O3A
3	D	902	ADP	C5'-O5'-PA-O3A
3	I	902	ADP	C4'-C5'-O5'-PA
3	C	902	ADP	C5'-O5'-PA-O2A
3	G	902	ADP	C5'-O5'-PA-O1A
3	H	902	ADP	C5'-O5'-PA-O1A
3	H	902	ADP	C5'-O5'-PA-O2A
2	G	901	IHP	C2-C1-O11-P1
2	G	901	IHP	C4-C3-O13-P3
2	K	901	IHP	C6-C1-O11-P1
3	E	902	ADP	PB-O3A-PA-O2A
3	F	902	ADP	PB-O3A-PA-O2A
3	H	902	ADP	O4'-C4'-C5'-O5'
2	A	901	IHP	C4-C3-O13-P3
2	C	901	IHP	C6-C1-O11-P1
2	K	901	IHP	C5-C4-O14-P4
2	L	901	IHP	C5-C6-O16-P6
2	B	901	IHP	C2-O12-P2-O22
2	E	901	IHP	C1-O11-P1-O21
2	H	901	IHP	C1-O11-P1-O21
2	I	901	IHP	C4-O14-P4-O24
2	I	901	IHP	C6-O16-P6-O26
2	J	901	IHP	C4-O14-P4-O24
2	K	901	IHP	C5-O15-P5-O25
2	L	901	IHP	C6-O16-P6-O26
3	L	902	ADP	PA-O3A-PB-O1B
3	L	902	ADP	C3'-C4'-C5'-O5'
3	C	902	ADP	PA-O3A-PB-O2B
3	L	902	ADP	PA-O3A-PB-O2B
2	A	901	IHP	C1-O11-P1-O41
2	A	901	IHP	C2-O12-P2-O32
2	B	901	IHP	C3-O13-P3-O43
2	B	901	IHP	C5-O15-P5-O45

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Mol	Chain	Res	Type	Atoms
2	D	901	IHP	C2-C1-O11-P1
2	D	901	IHP	C2-O12-P2-O32
2	D	901	IHP	C6-O16-P6-O36
2	E	901	IHP	C1-O11-P1-O41
2	E	901	IHP	C3-O13-P3-O33
2	E	901	IHP	C6-O16-P6-O46
2	F	901	IHP	C2-O12-P2-O42
2	G	901	IHP	C1-C2-O12-P2
2	G	901	IHP	C2-C3-O13-P3
2	H	901	IHP	C2-O12-P2-O32
2	H	901	IHP	C3-O13-P3-O33
2	I	901	IHP	C3-C2-O12-P2
2	I	901	IHP	C1-O11-P1-O41
2	I	901	IHP	C4-O14-P4-O34
2	J	901	IHP	C4-O14-P4-O44
2	J	901	IHP	C5-O15-P5-O45
2	K	901	IHP	C4-O14-P4-O34
2	L	901	IHP	C1-O11-P1-O41
2	L	901	IHP	C2-O12-P2-O32
3	A	902	ADP	C5'-O5'-PA-O3A
3	F	902	ADP	C5'-O5'-PA-O3A
3	I	902	ADP	C5'-O5'-PA-O3A
3	D	902	ADP	O4'-C4'-C5'-O5'
3	E	902	ADP	PB-O3A-PA-O1A
3	A	902	ADP	C5'-O5'-PA-O1A
3	D	902	ADP	C5'-O5'-PA-O1A
3	K	902	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

17 monomers are involved in 51 short contacts:

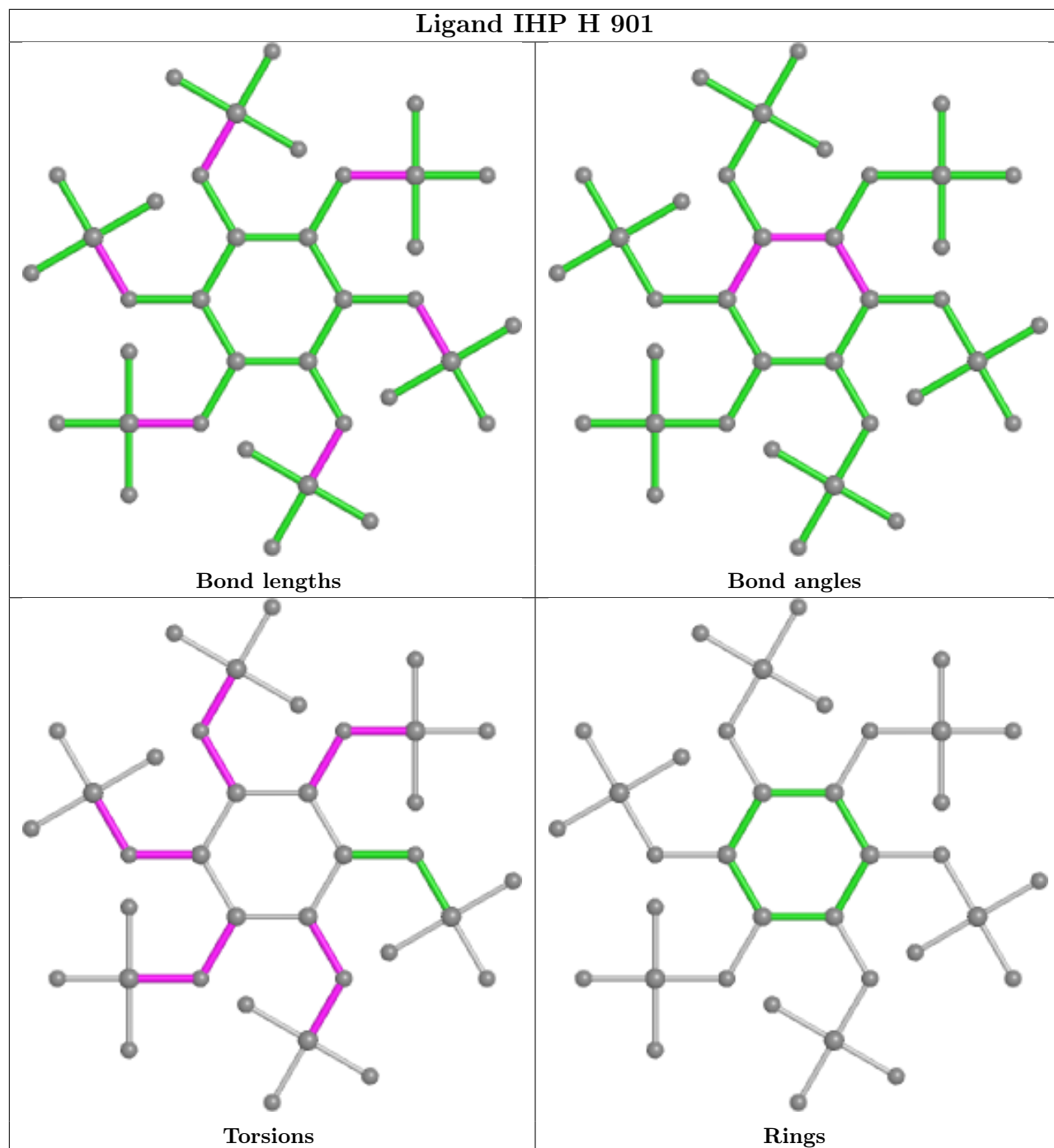
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	901	IHP	2	0
3	G	902	ADP	1	0
3	J	902	ADP	3	0
3	B	902	ADP	4	0
2	L	901	IHP	1	0
3	D	902	ADP	6	0
3	F	902	ADP	4	0
2	K	901	IHP	1	0
2	I	901	IHP	2	0
3	H	902	ADP	3	0

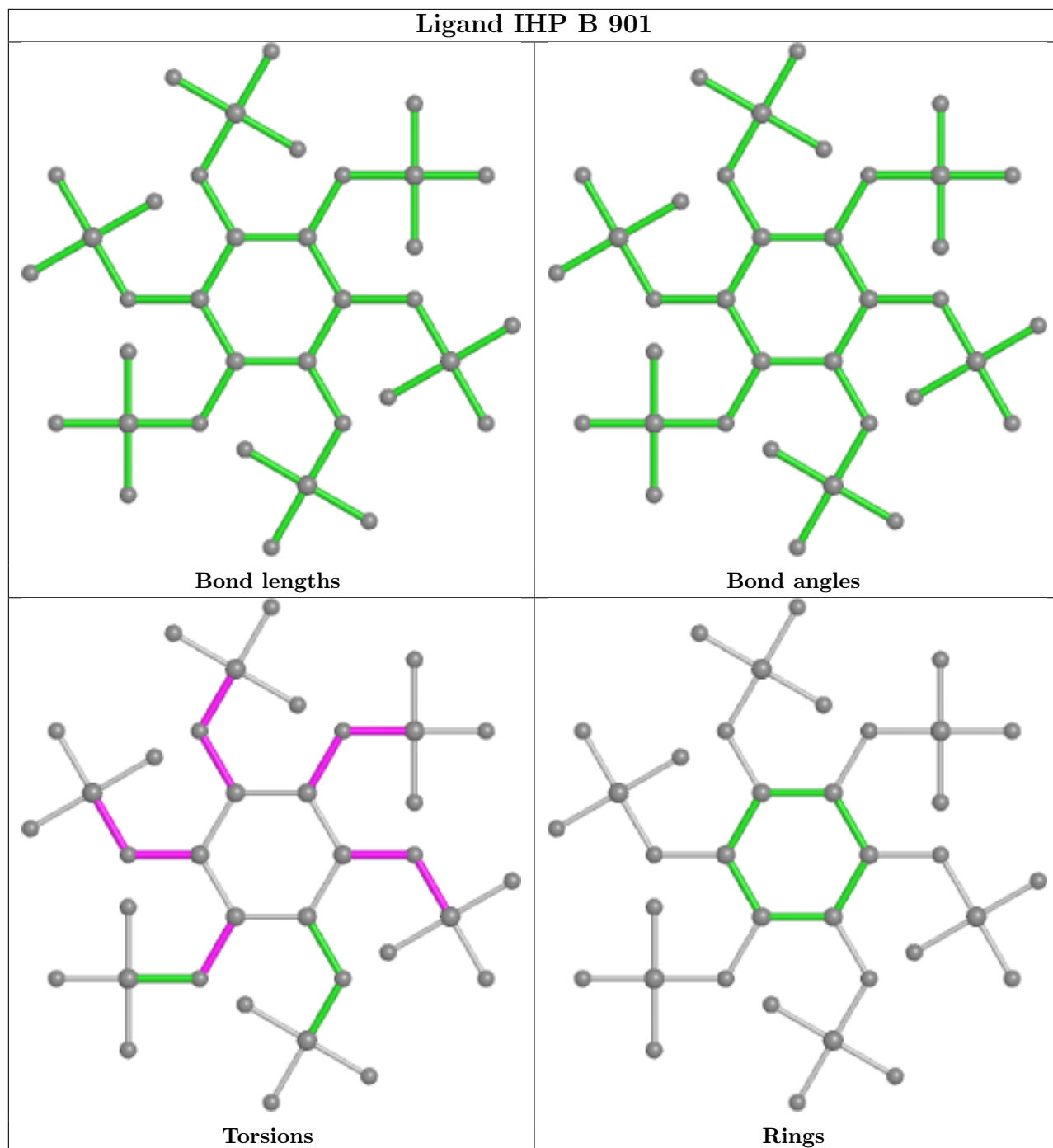
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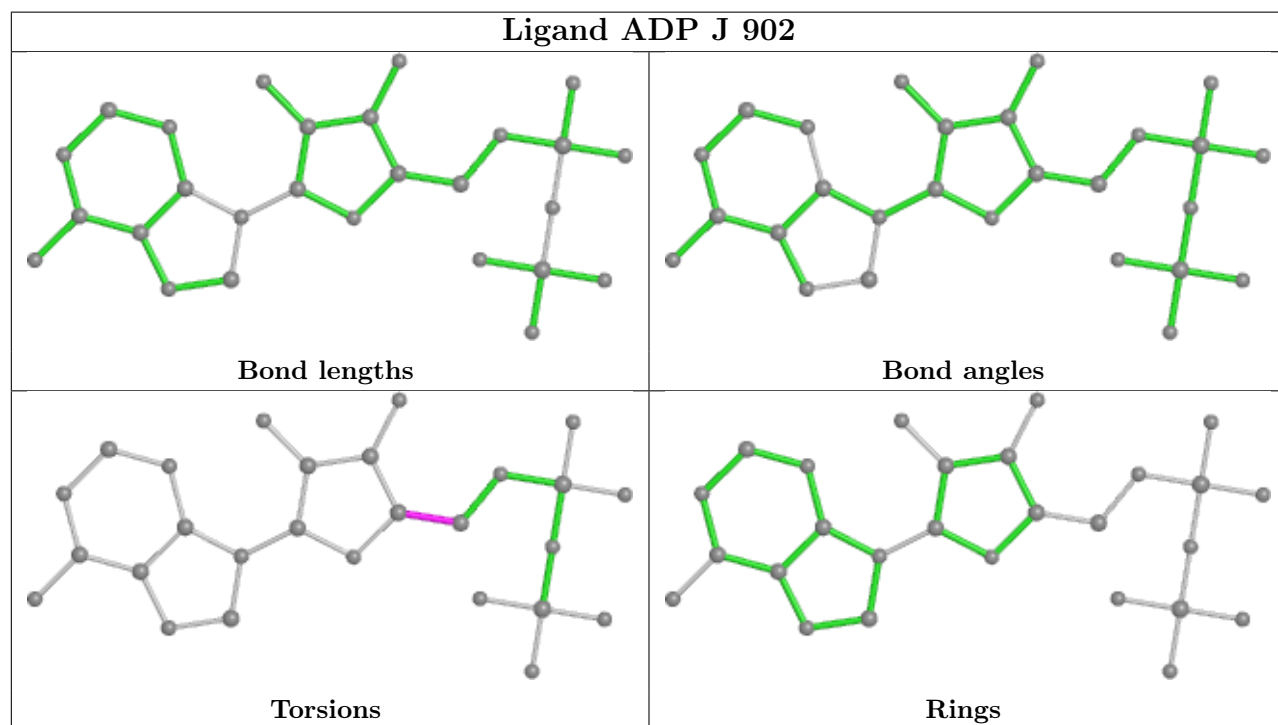
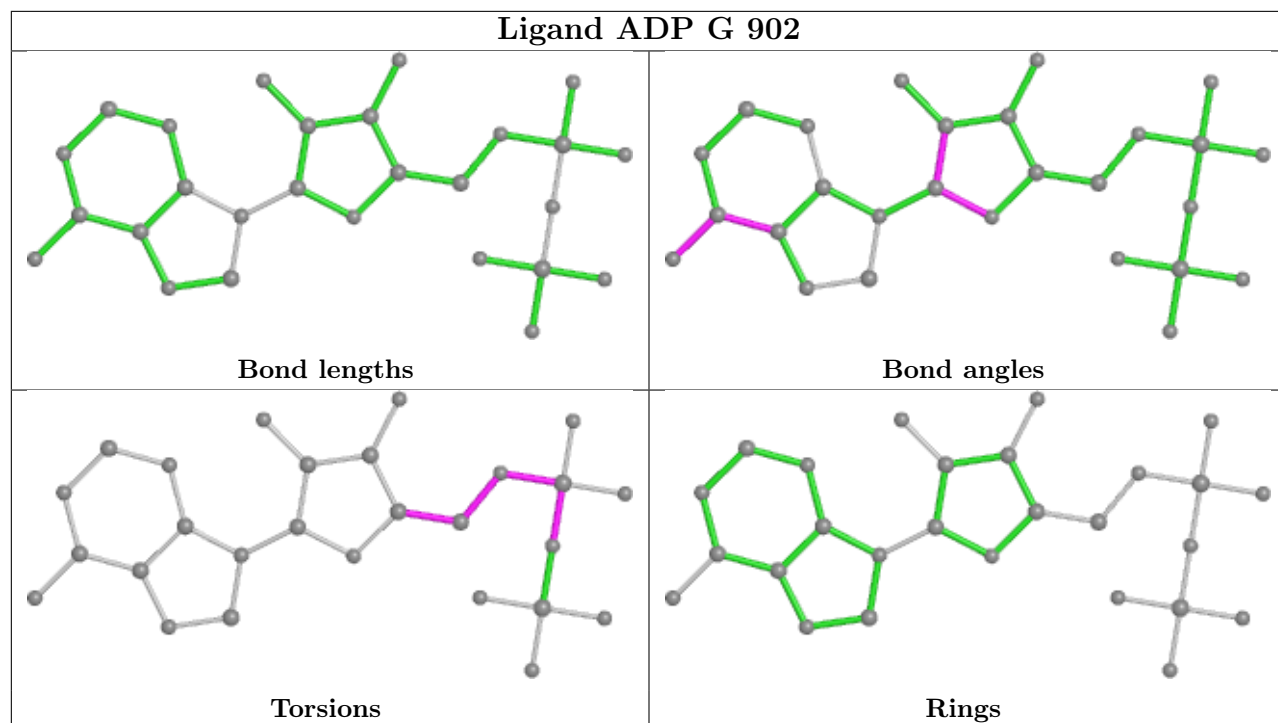
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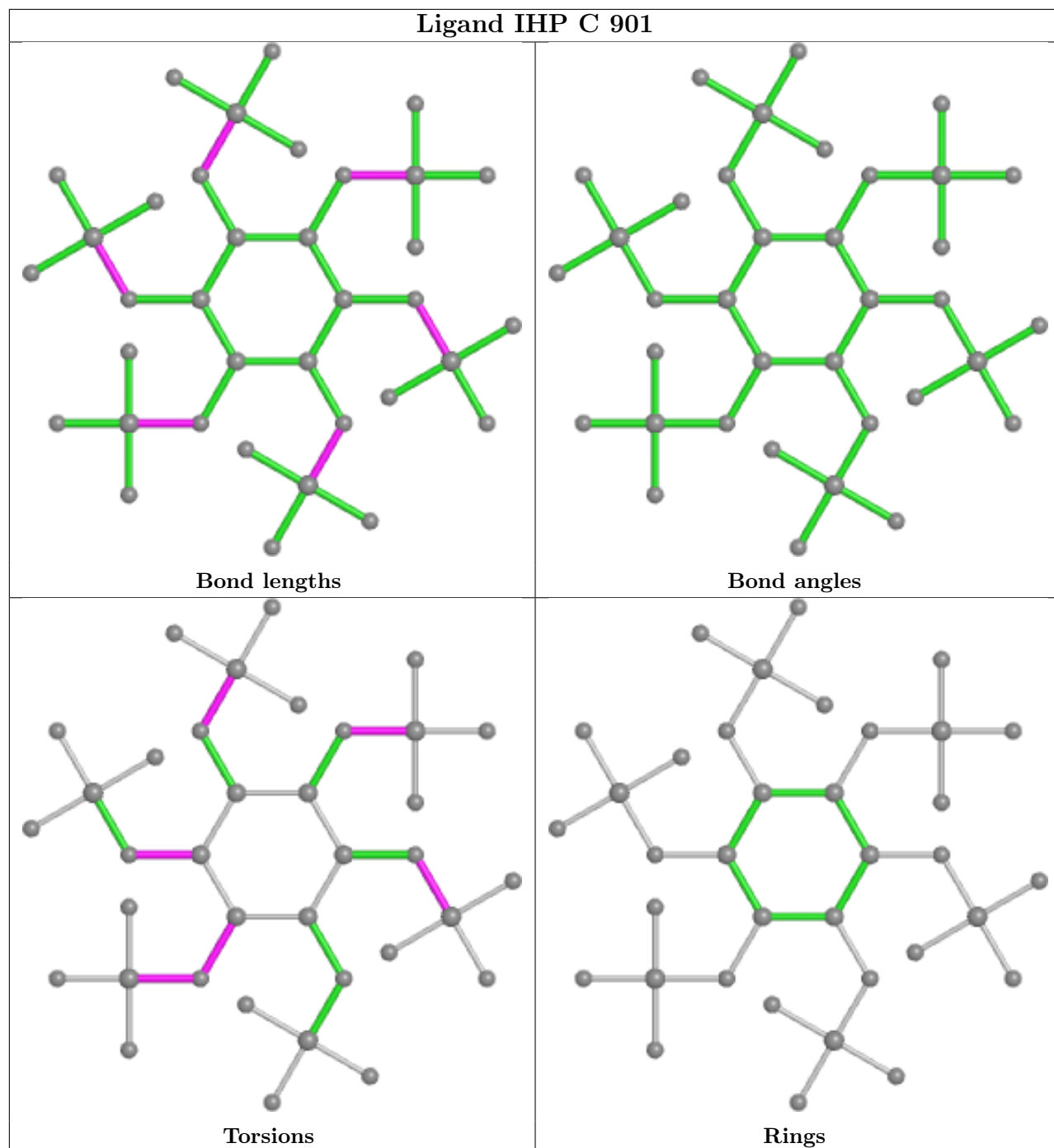
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	902	ADP	3	0
3	C	902	ADP	3	0
3	L	902	ADP	7	0
3	K	902	ADP	4	0
3	A	902	ADP	5	0
2	D	901	IHP	1	0
3	E	902	ADP	1	0

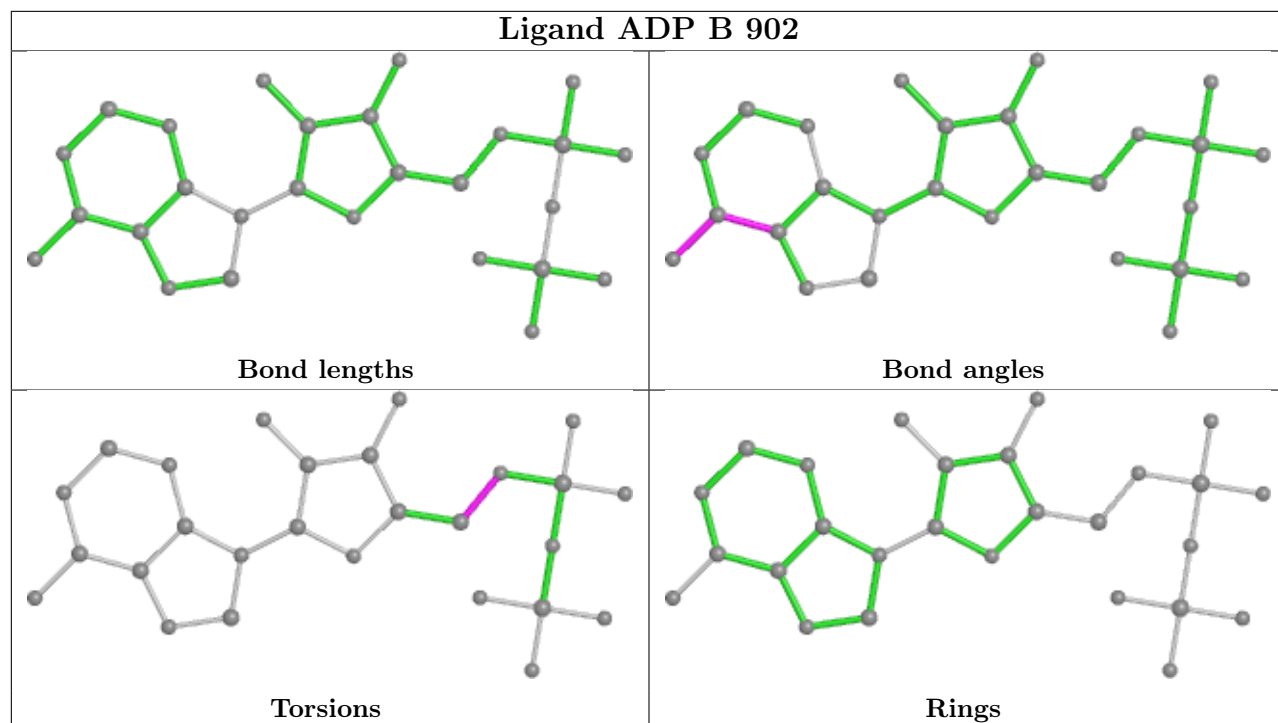
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

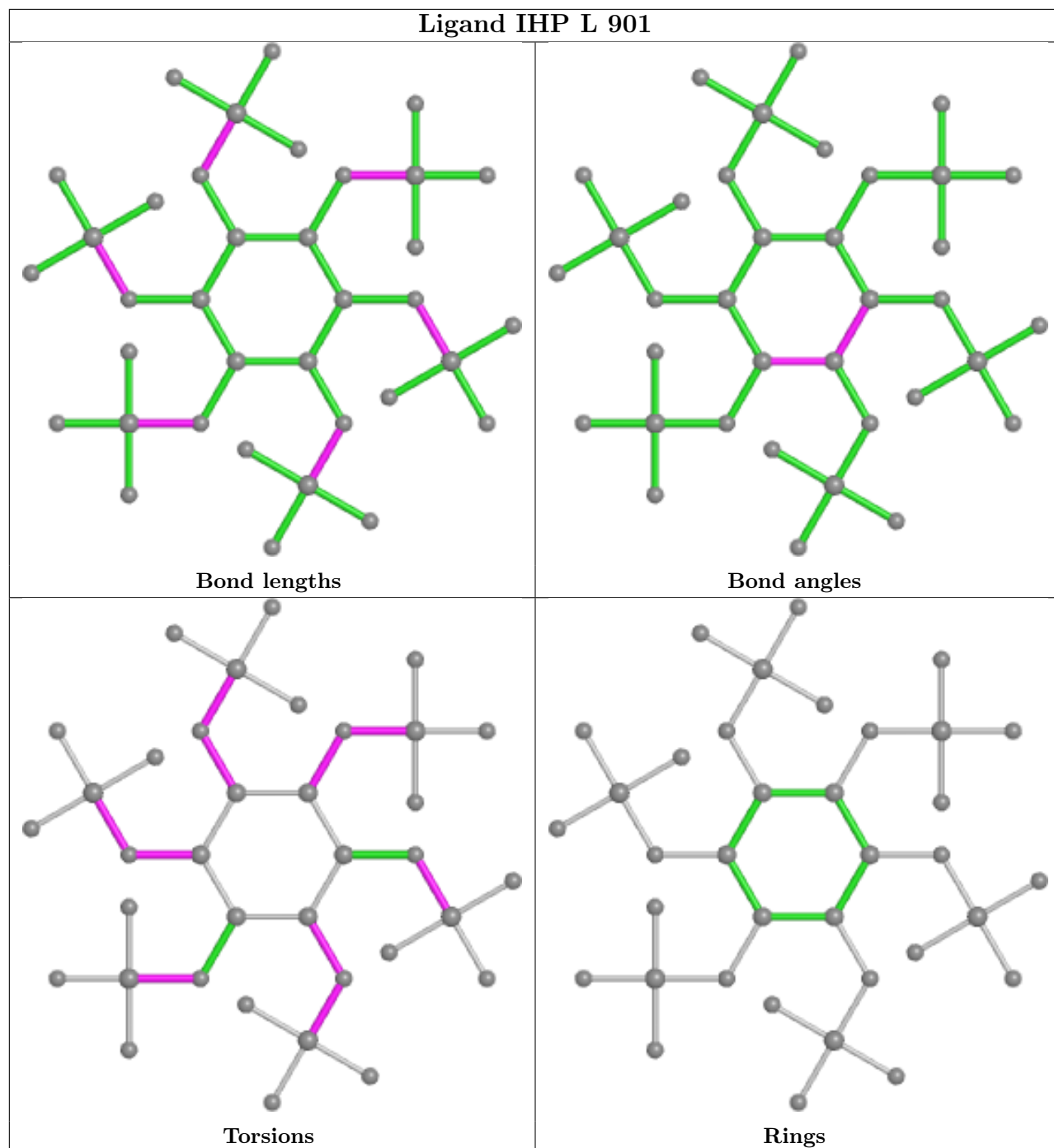


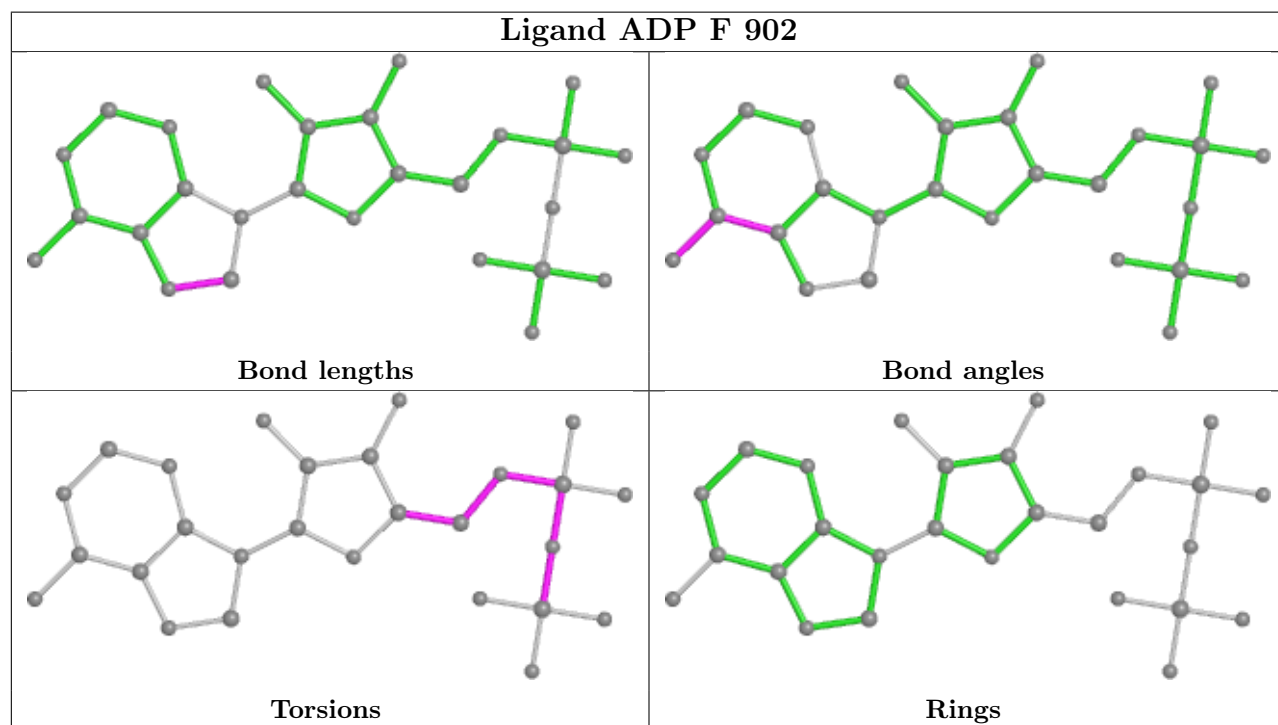
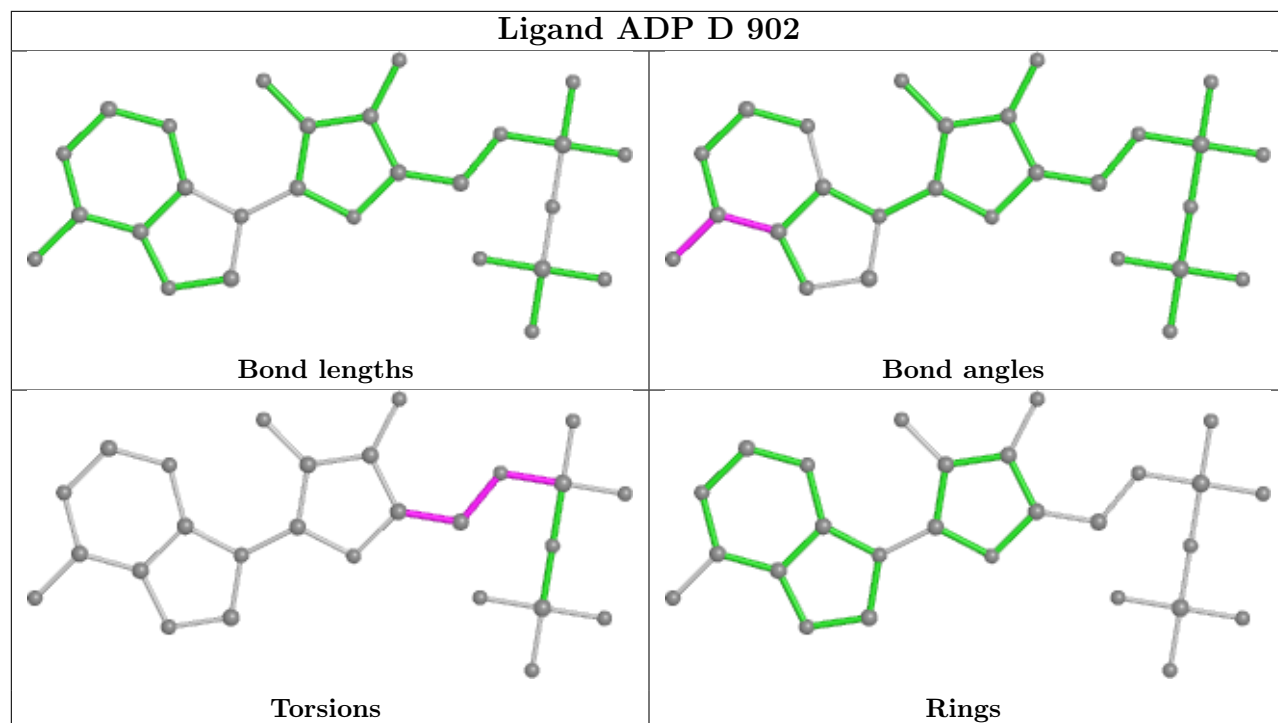


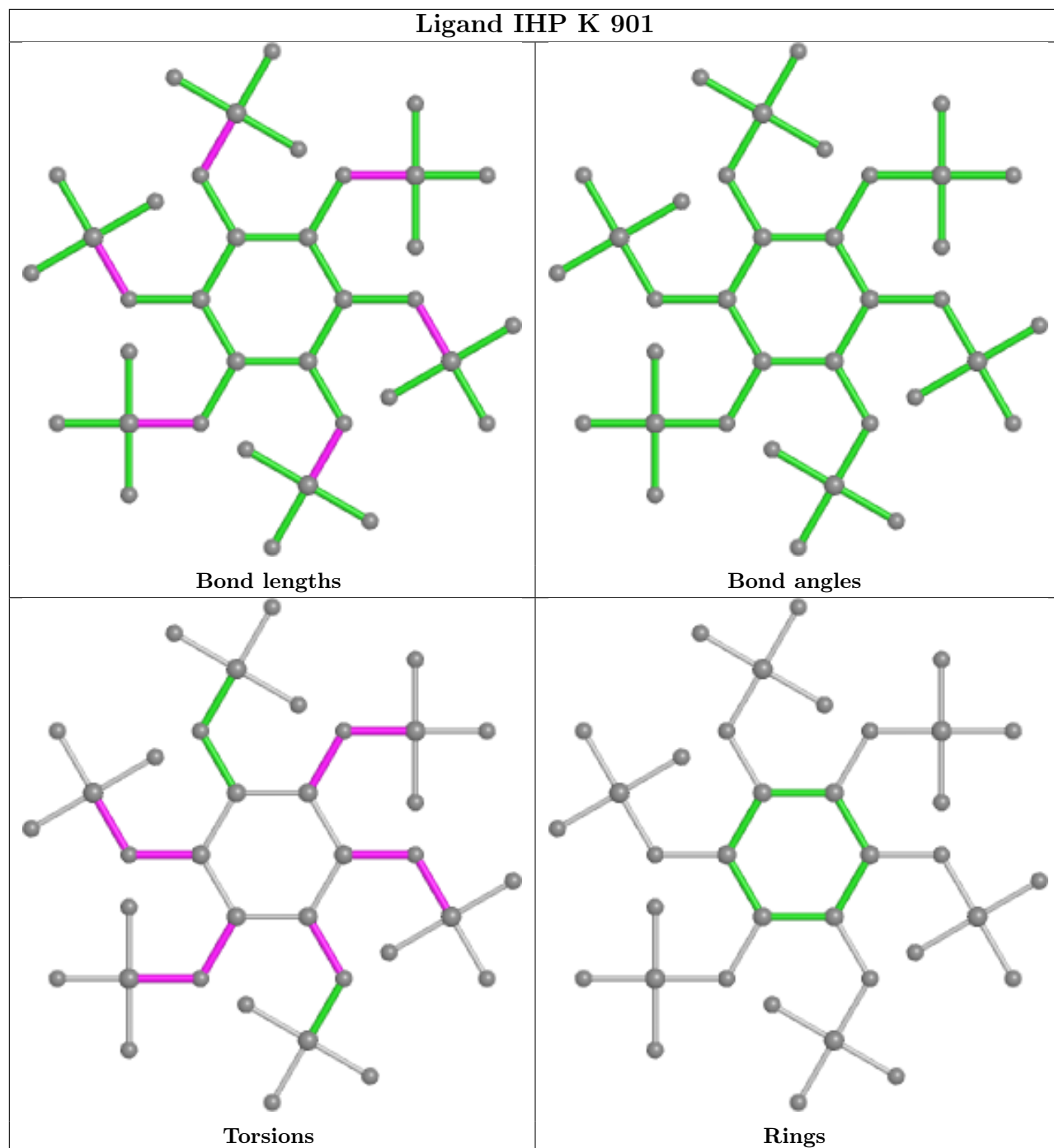


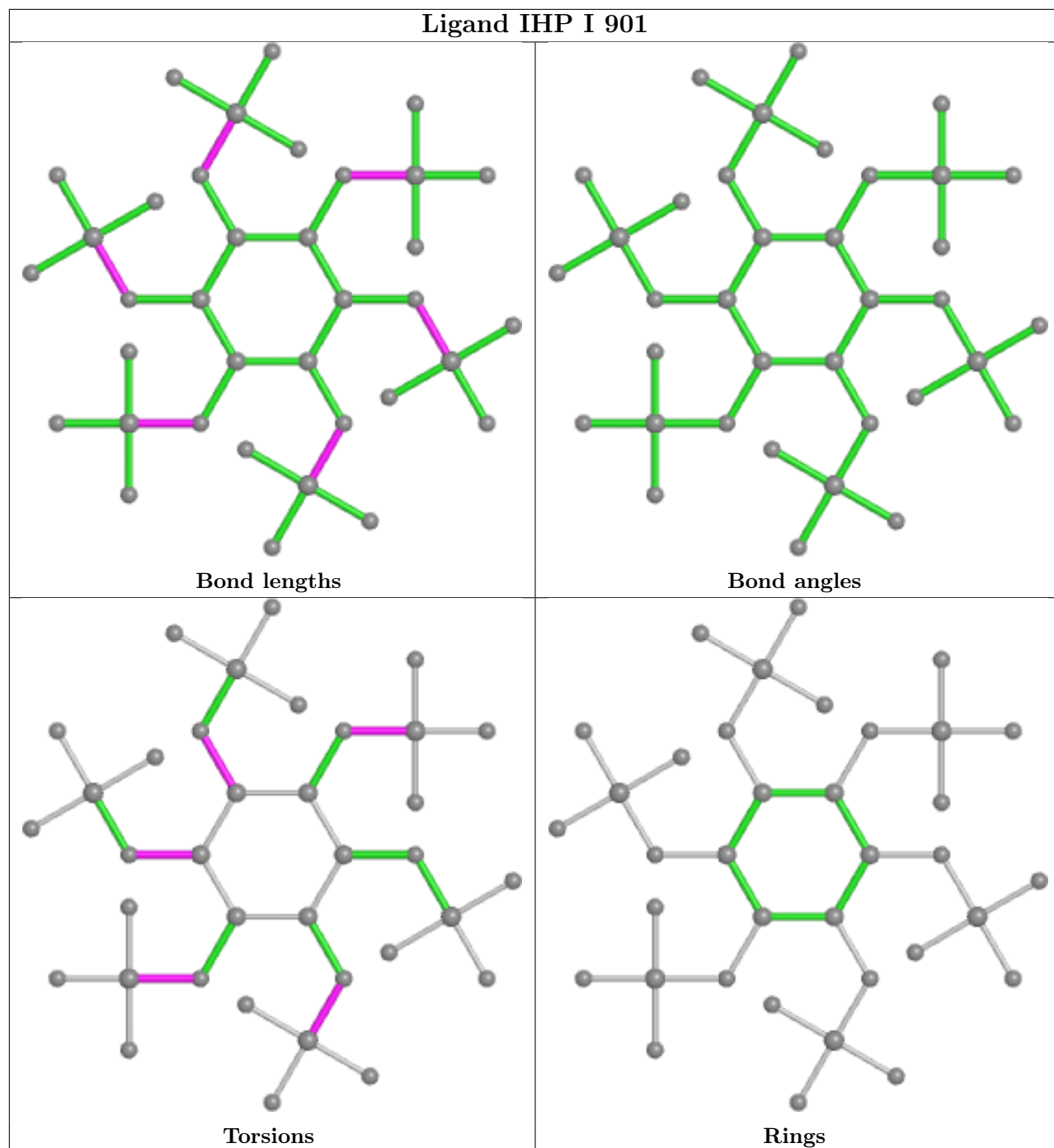


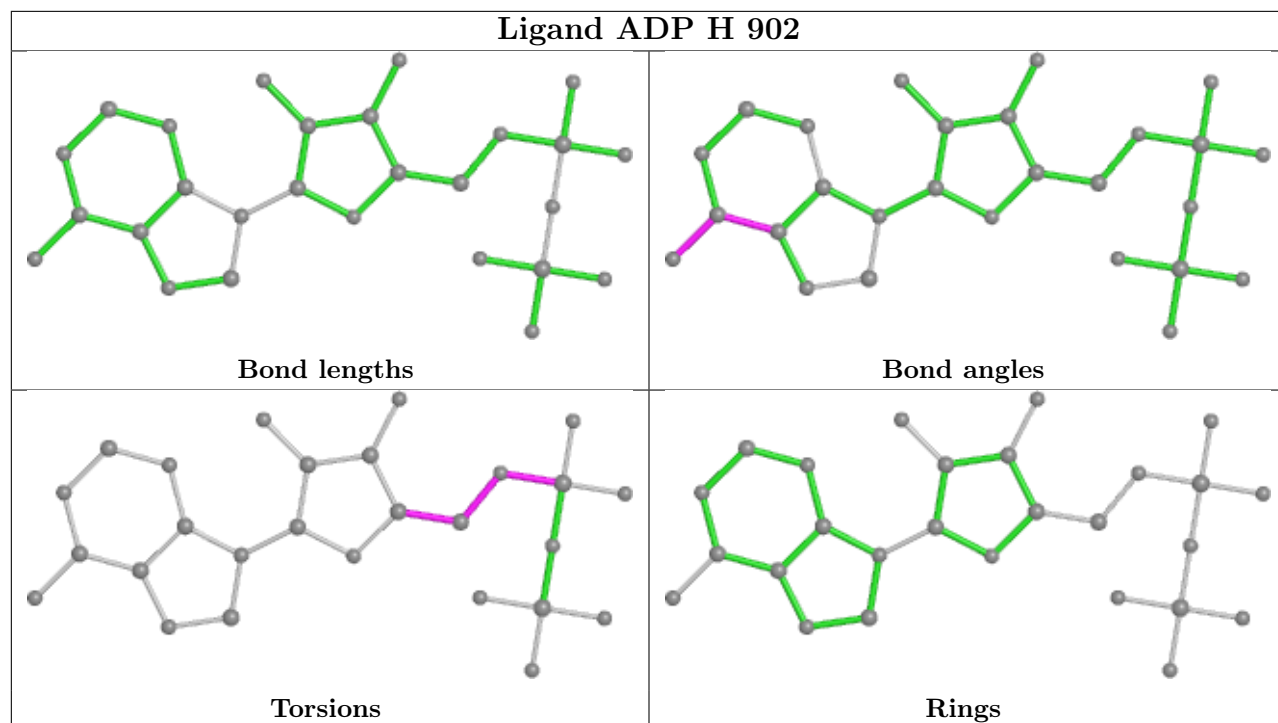


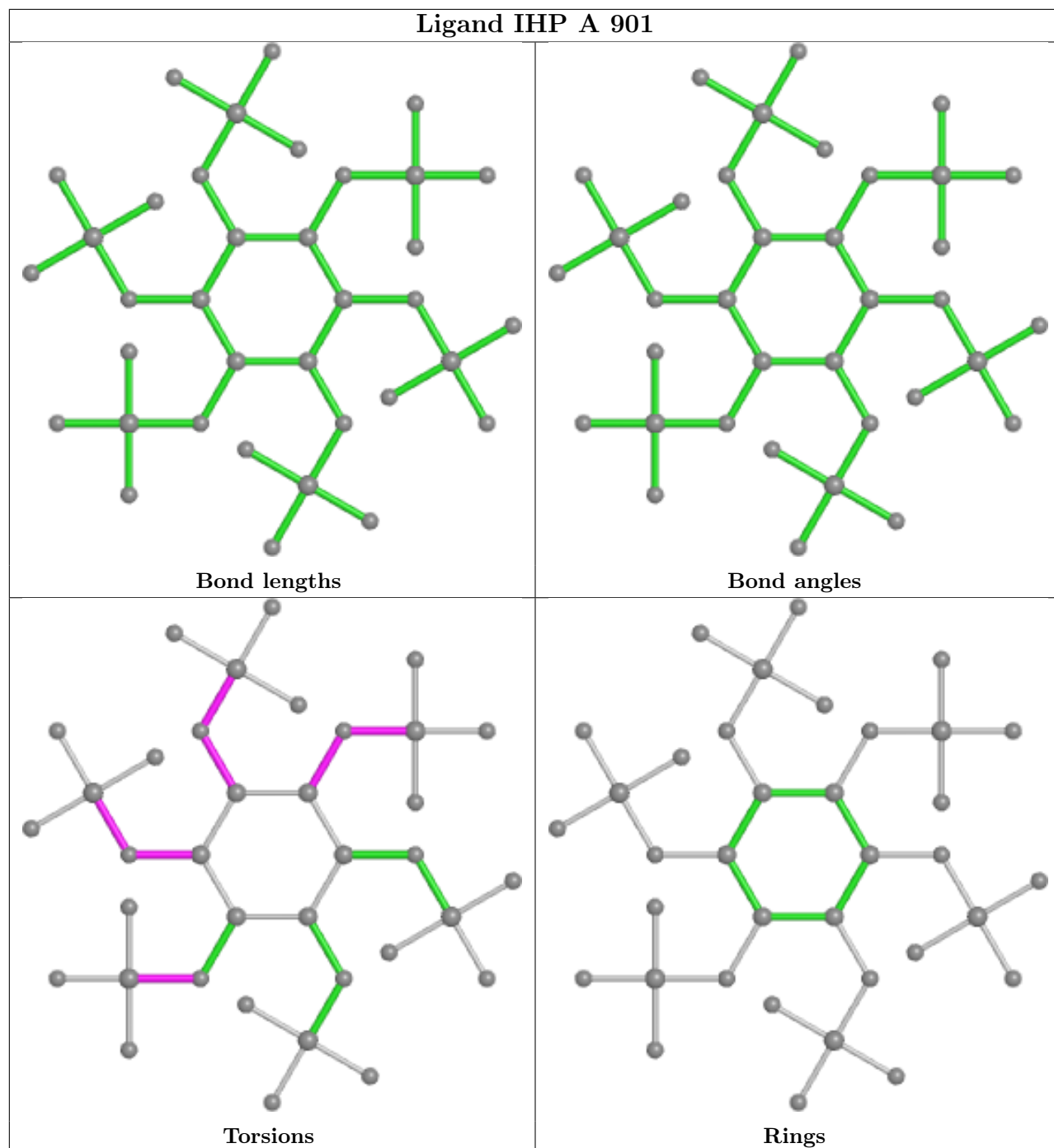


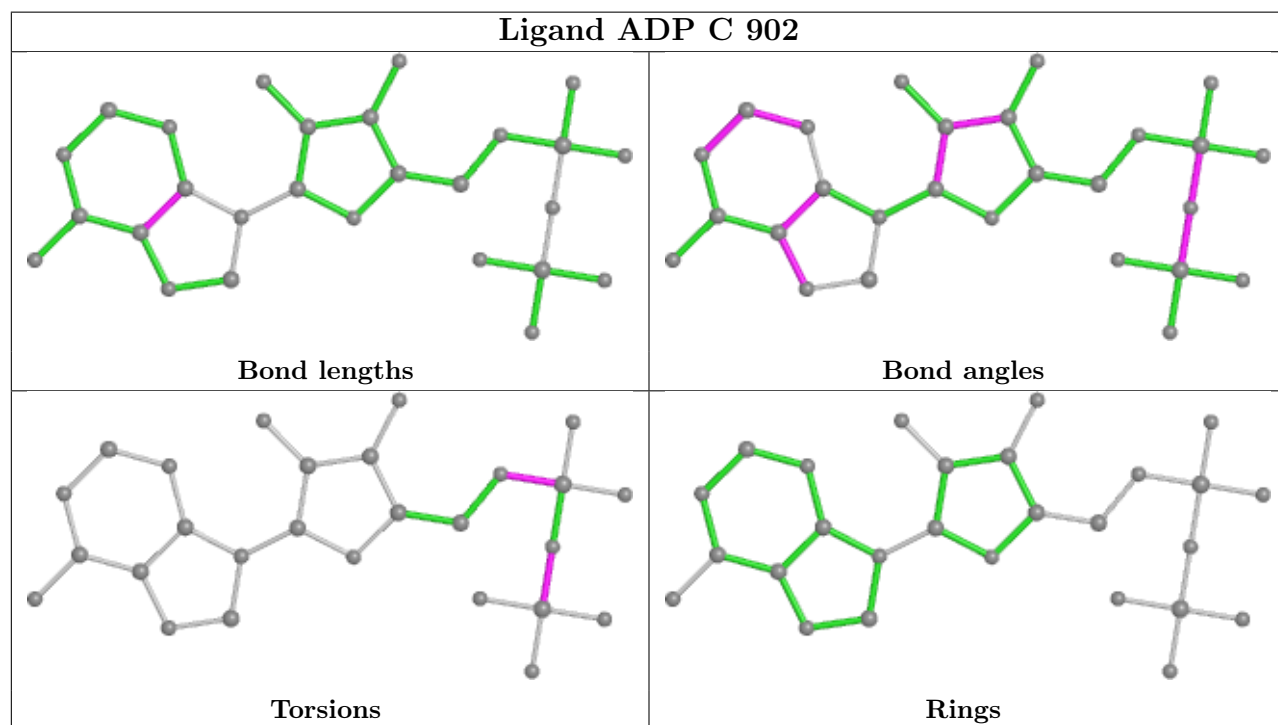
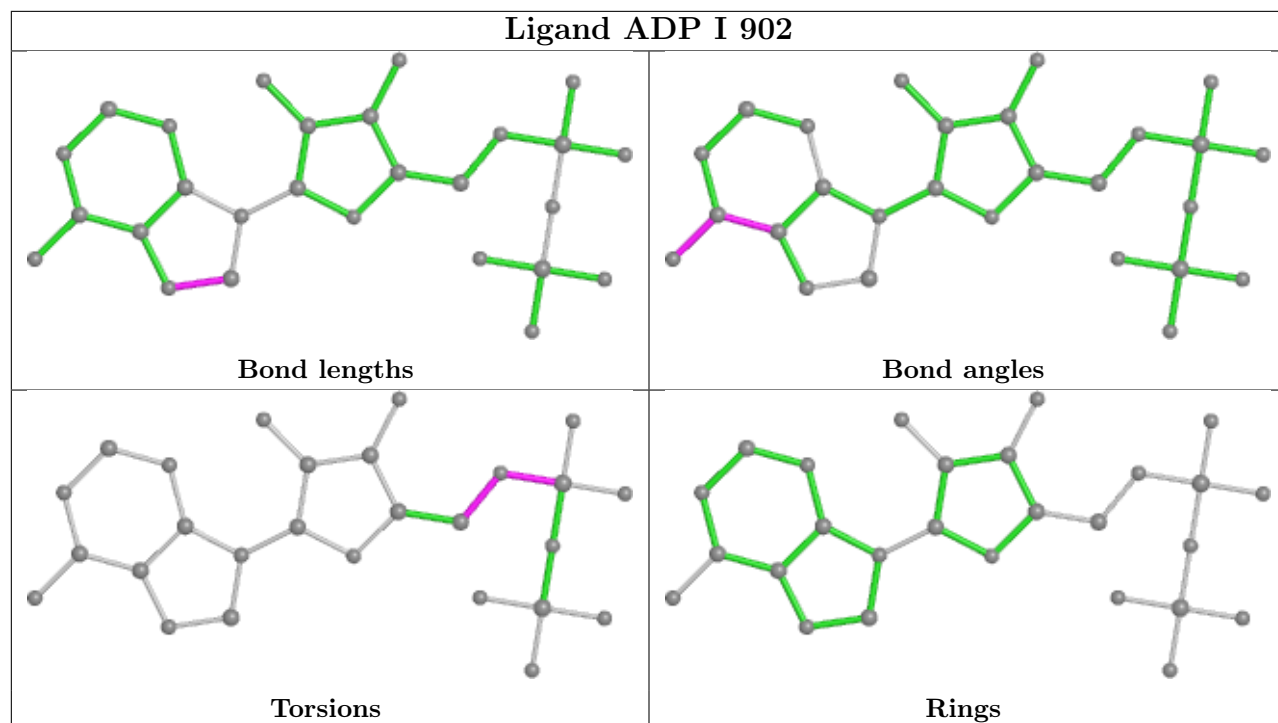


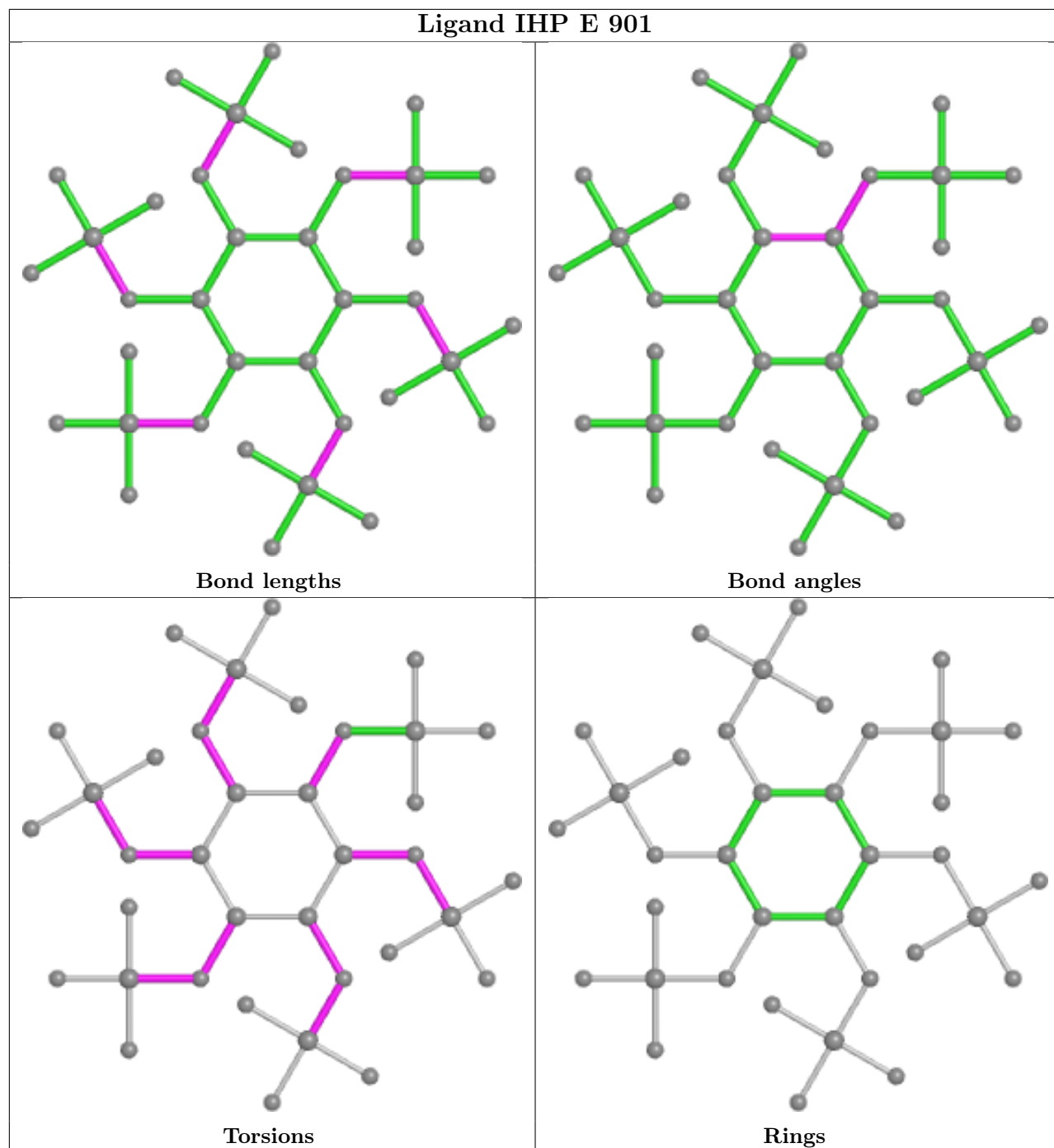


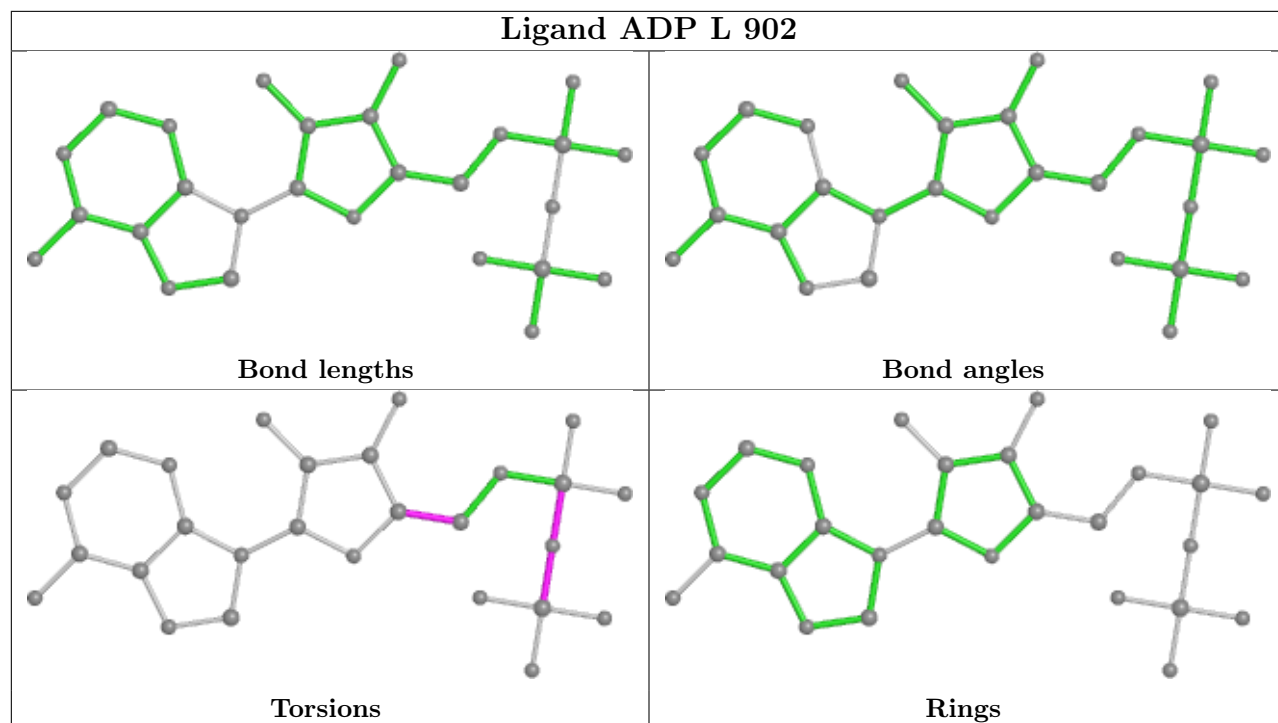


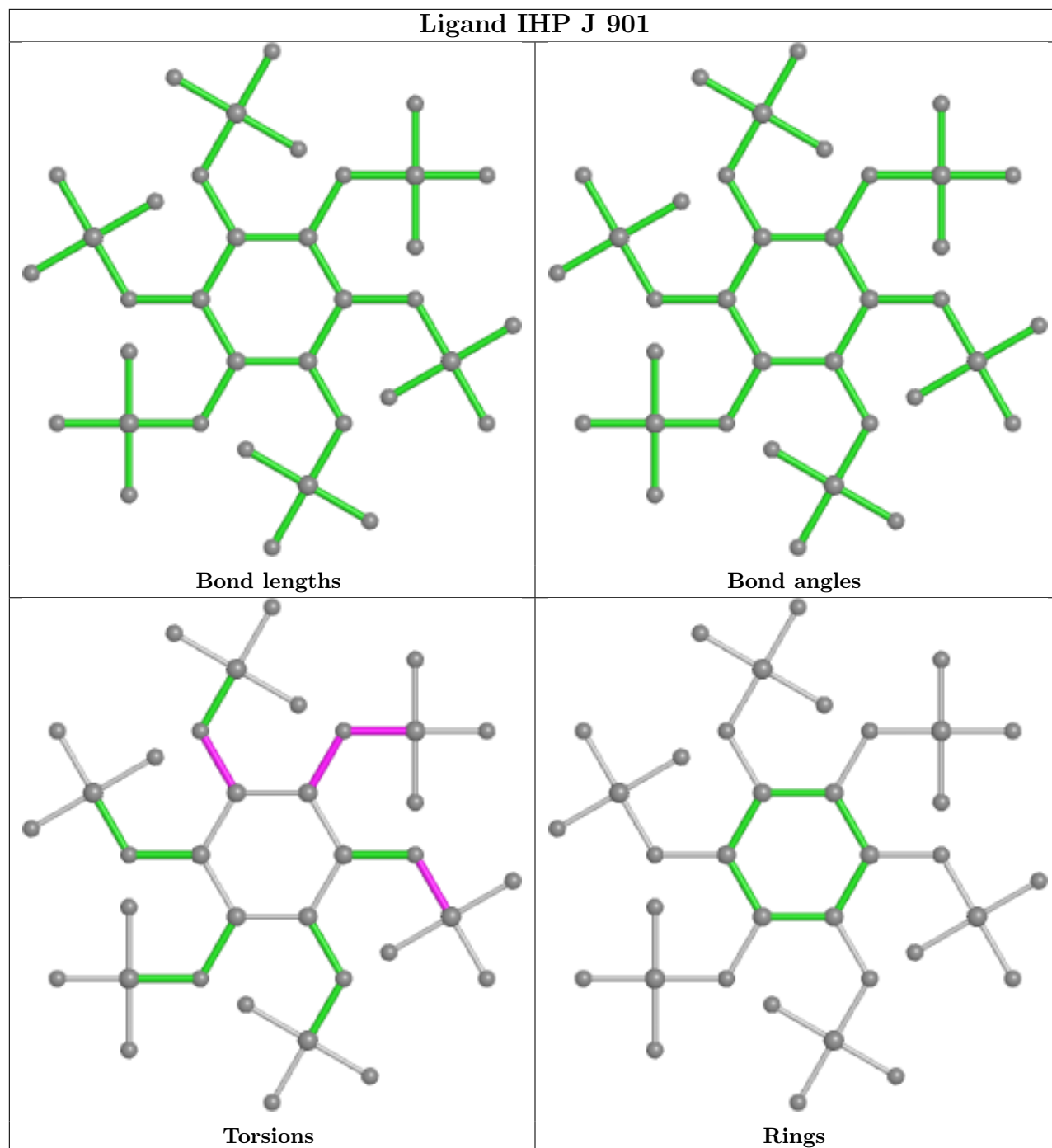


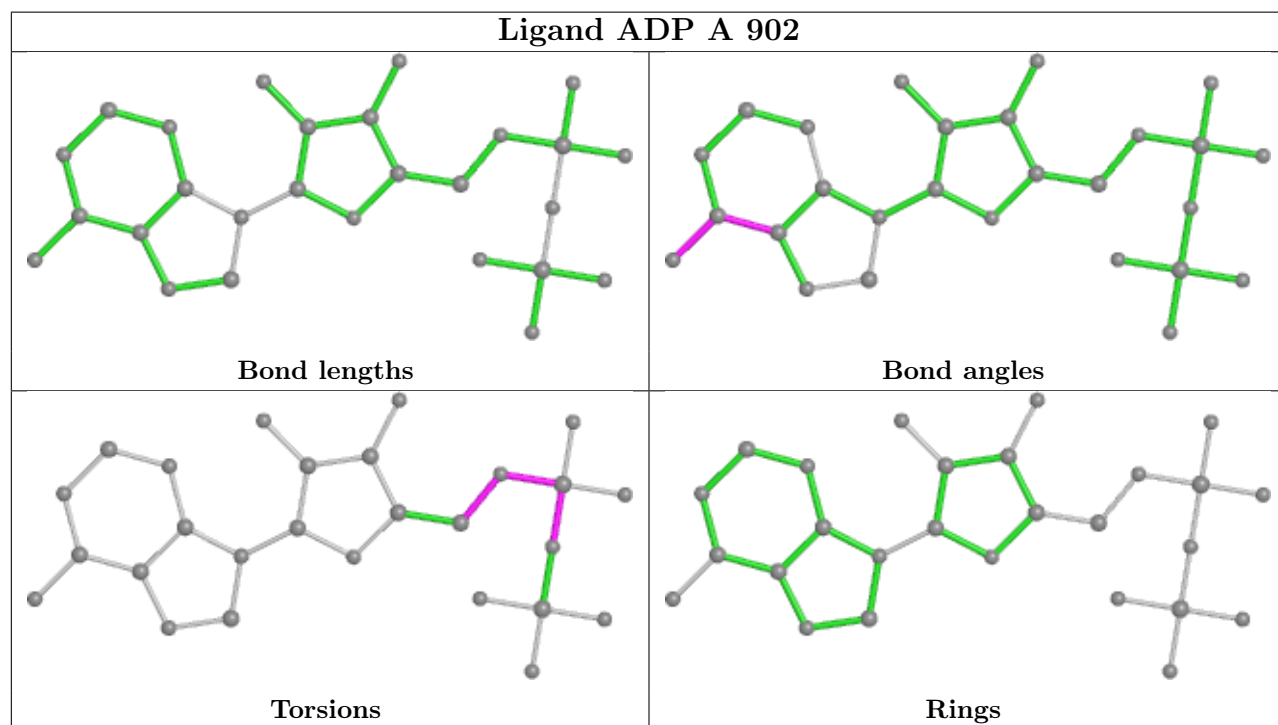
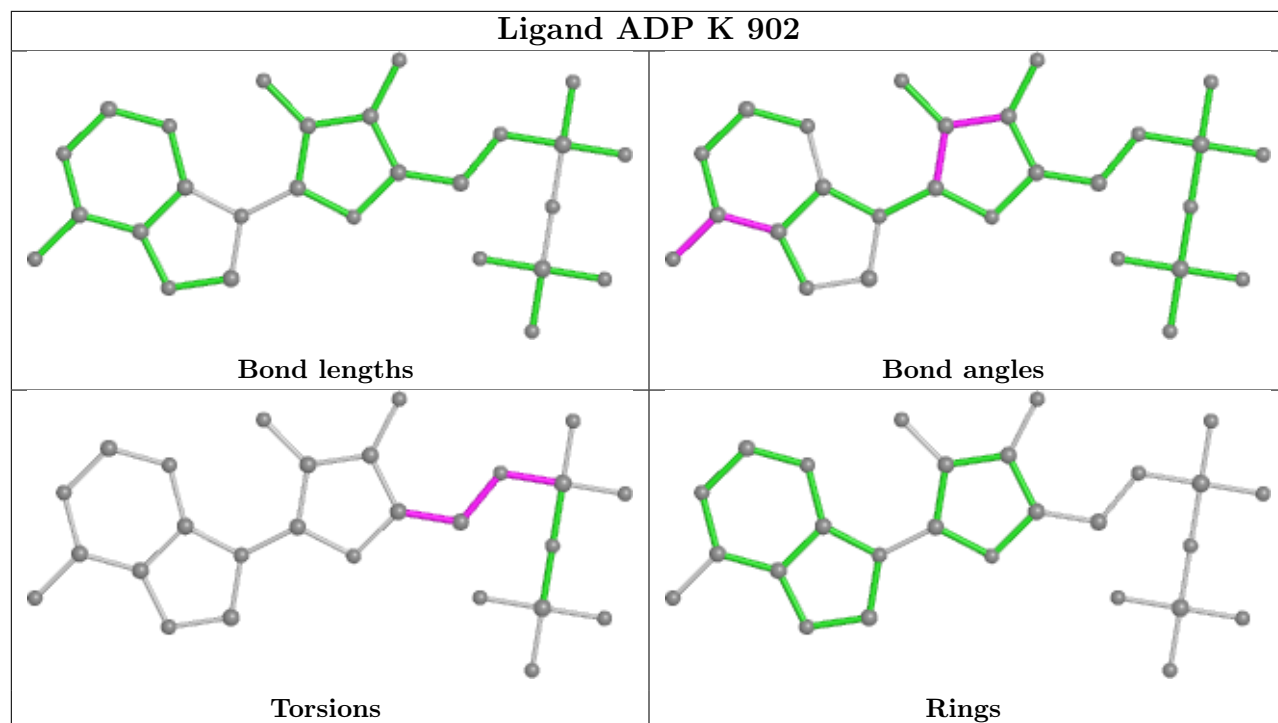


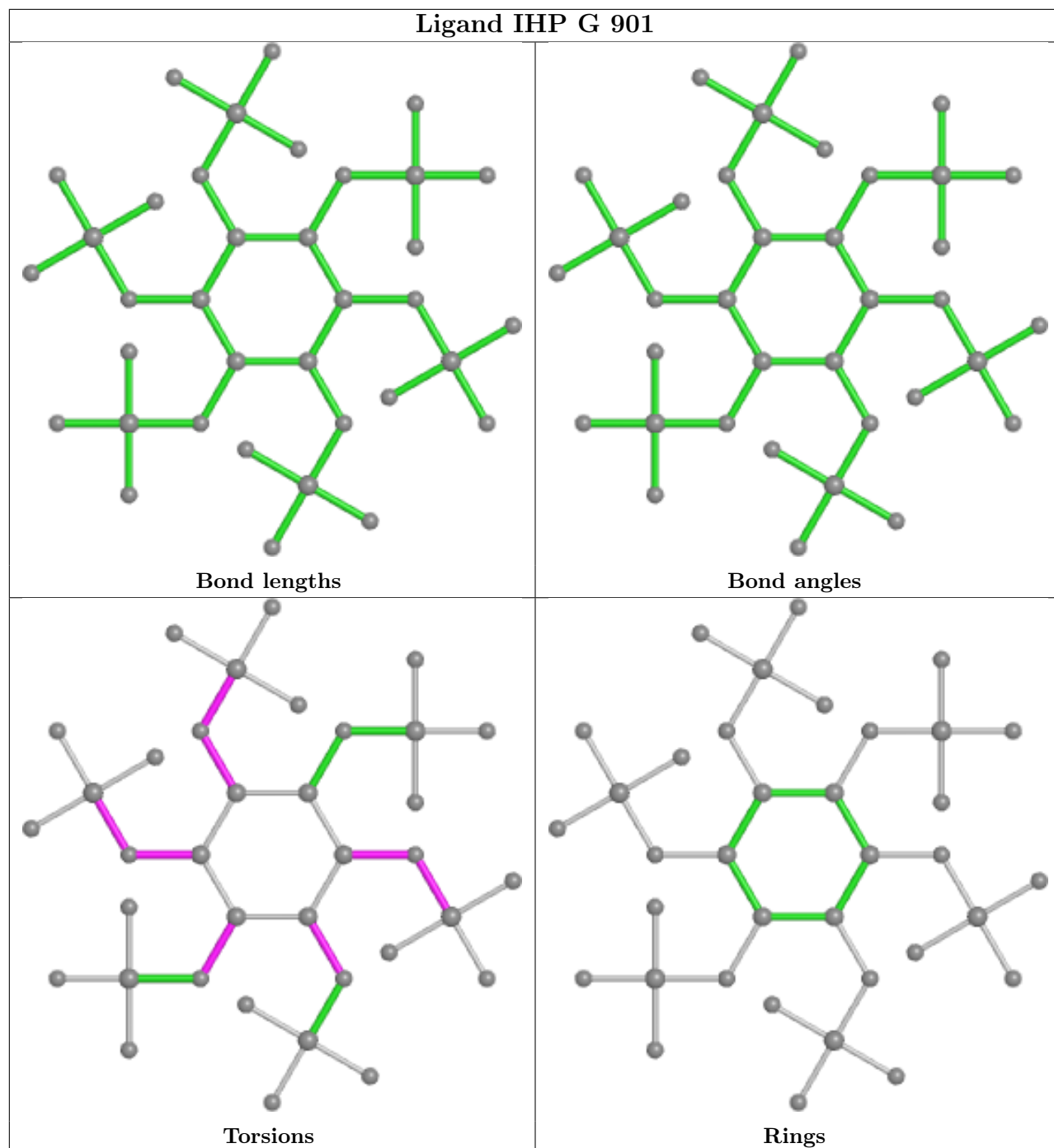


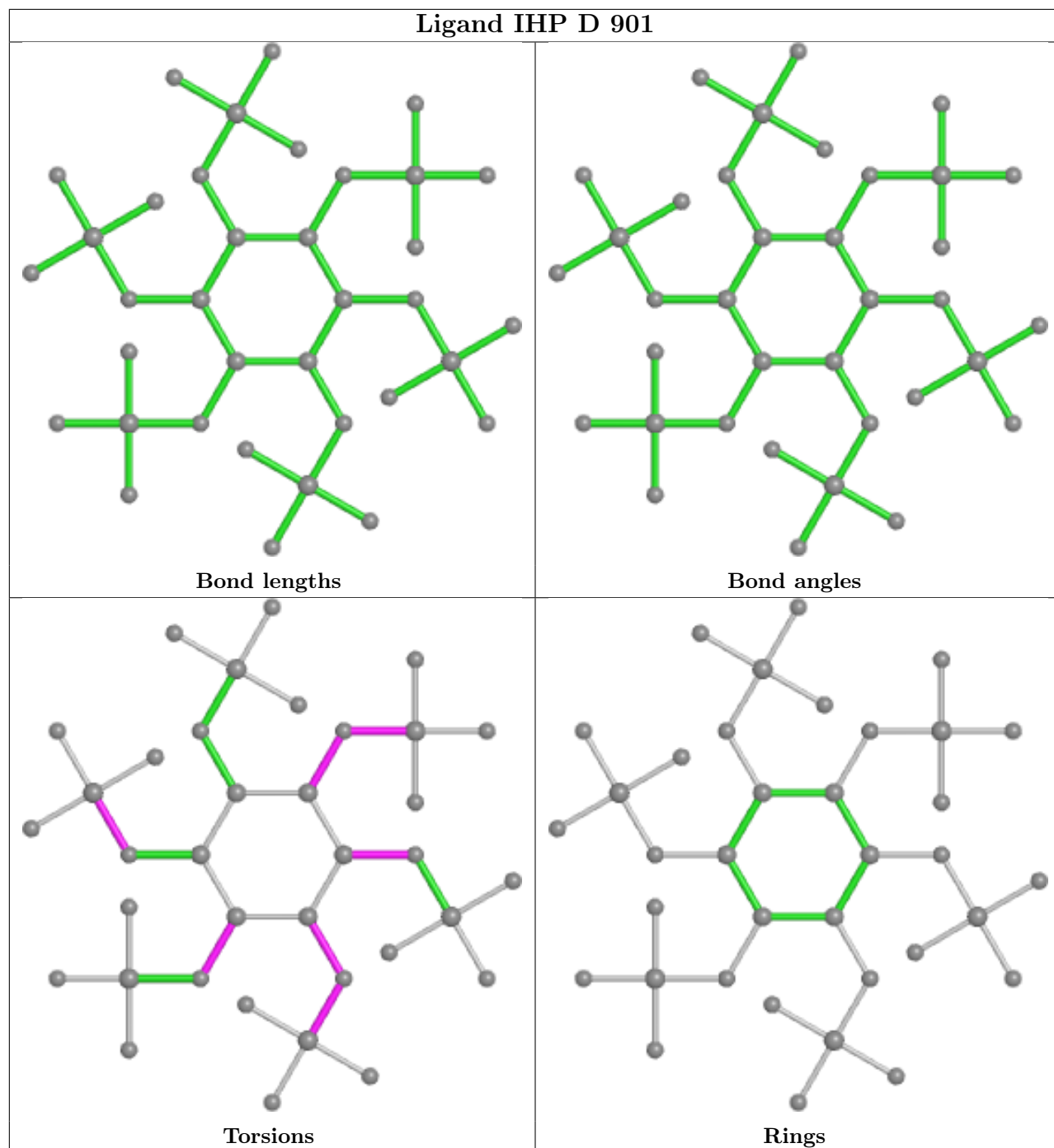


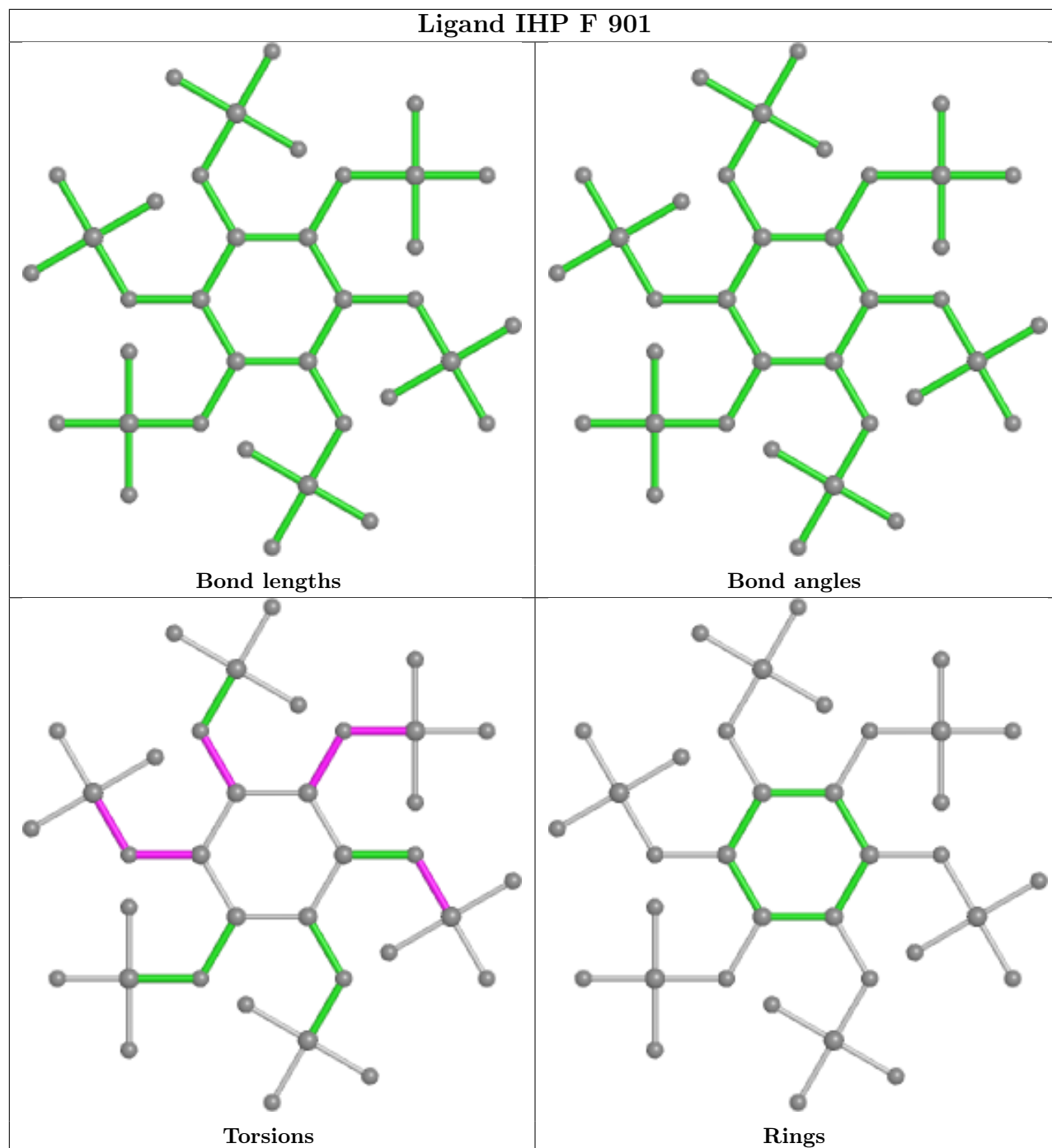


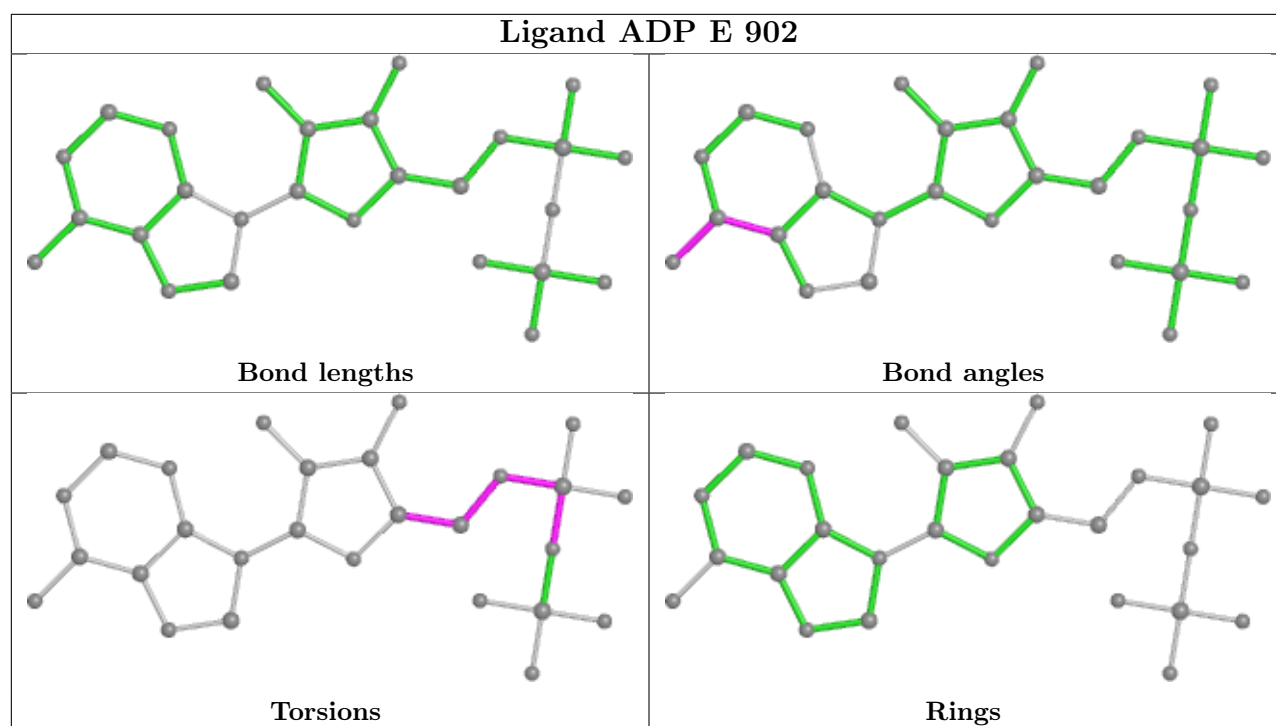












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.