Full wwPDB EM Validation Report ⓘ

May 15, 2024 – 09:46 PM 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:

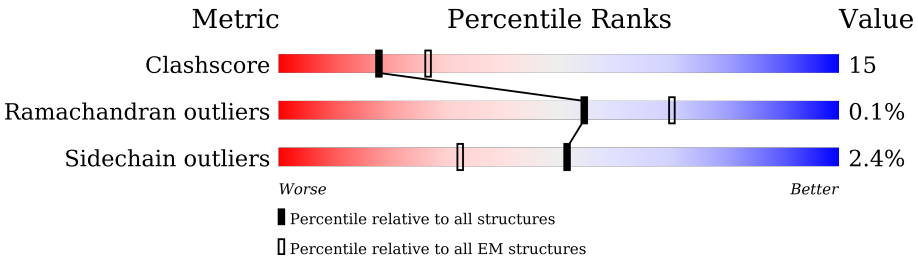
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	885	8% 69% 30%
1	B	885	6% 67% 32%
1	C	885	9% 68% 31%
1	D	885	9% 74% 26%
1	E	885	7% 66% 32%
1	F	885	8% 69% 29%
1	G	885	9% 73% 26%
1	H	885	7% 72% 27%

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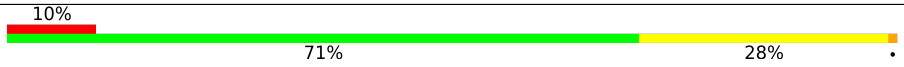
Mol	Chain	Length	Quality of chain
1	I	885	
1	J	885	
1	K	885	
1	L	885	

2 Entry composition (i)

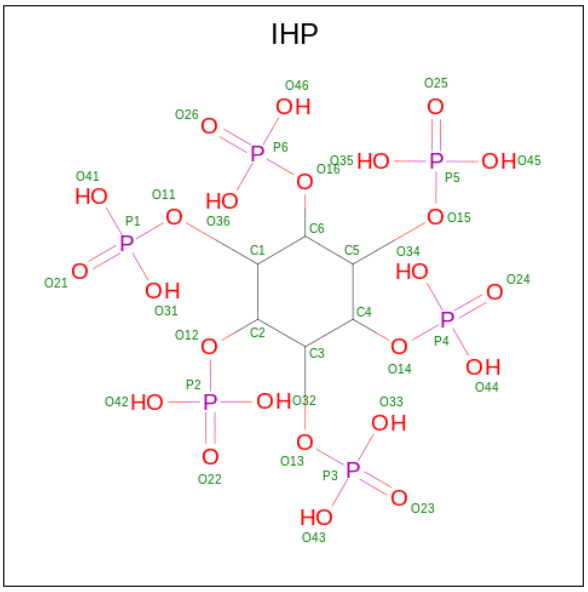
There are 3 unique types of molecules in this entry. The entry contains 86208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

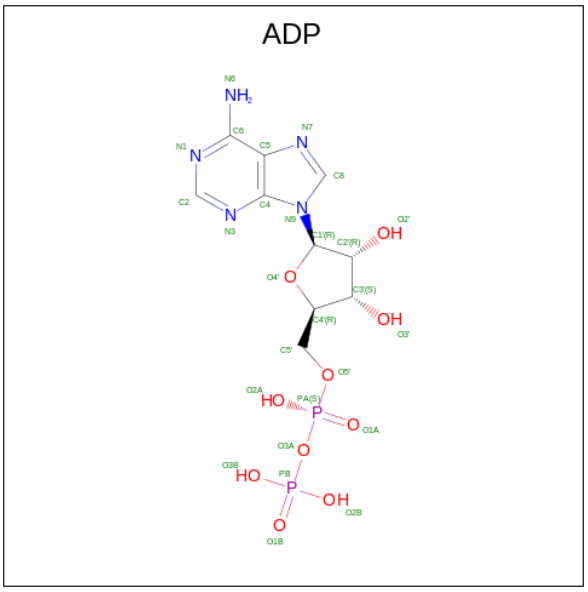
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	B	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	C	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	D	885	Total	C	N	O	S	0	0
			7121	4544	1237	1308	32		
1	E	885	Total	C	N	O	S	0	0
			7121	4544	1237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

- 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
2	A	1	Total	C	O	P	0
			36	6	24	6	
2	B	1	Total	C	O	P	0
			36	6	24	6	
2	C	1	Total	C	O	P	0
			36	6	24	6	
2	D	1	Total	C	O	P	0
			36	6	24	6	
2	E	1	Total	C	O	P	0
			36	6	24	6	
2	F	1	Total	C	O	P	0
			36	6	24	6	
2	G	1	Total	C	O	P	0
			36	6	24	6	
2	H	1	Total	C	O	P	0
			36	6	24	6	
2	I	1	Total	C	O	P	0
			36	6	24	6	
2	J	1	Total	C	O	P	0
			36	6	24	6	
2	K	1	Total	C	O	P	0
			36	6	24	6	
2	L	1	Total	C	O	P	0
			36	6	24	6	

- 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).



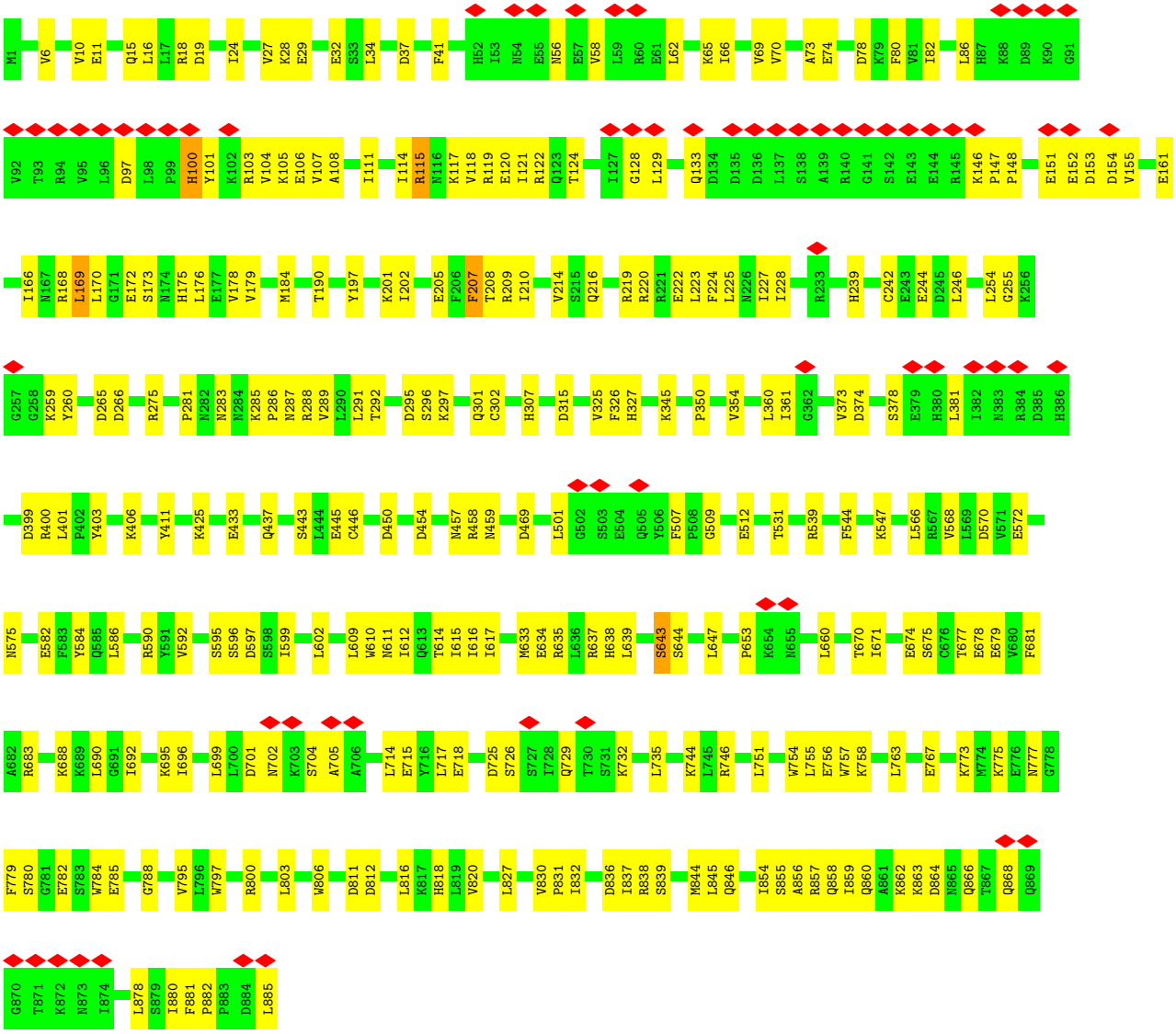
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

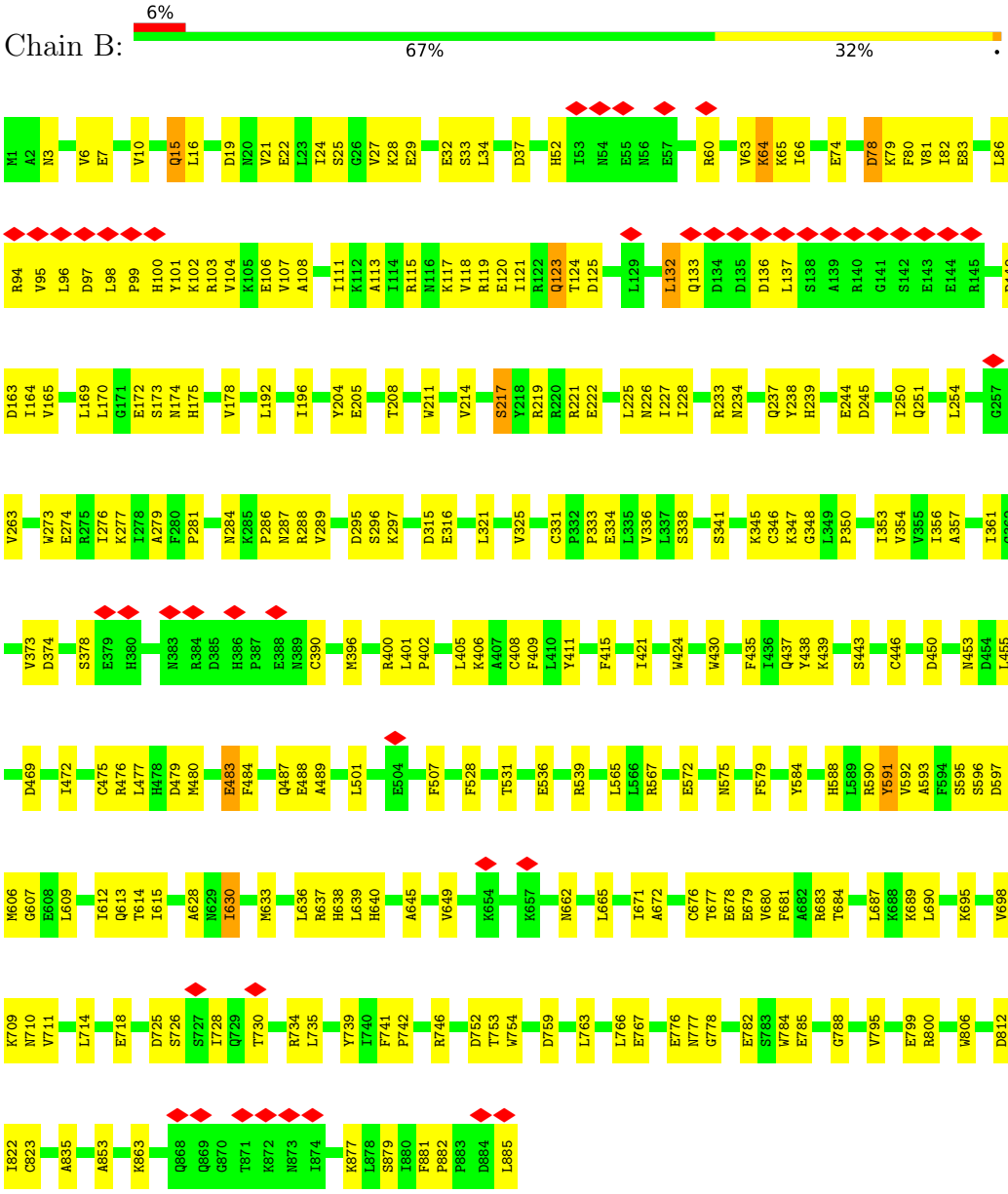
- Molecule 1: NRC2

Chain A:



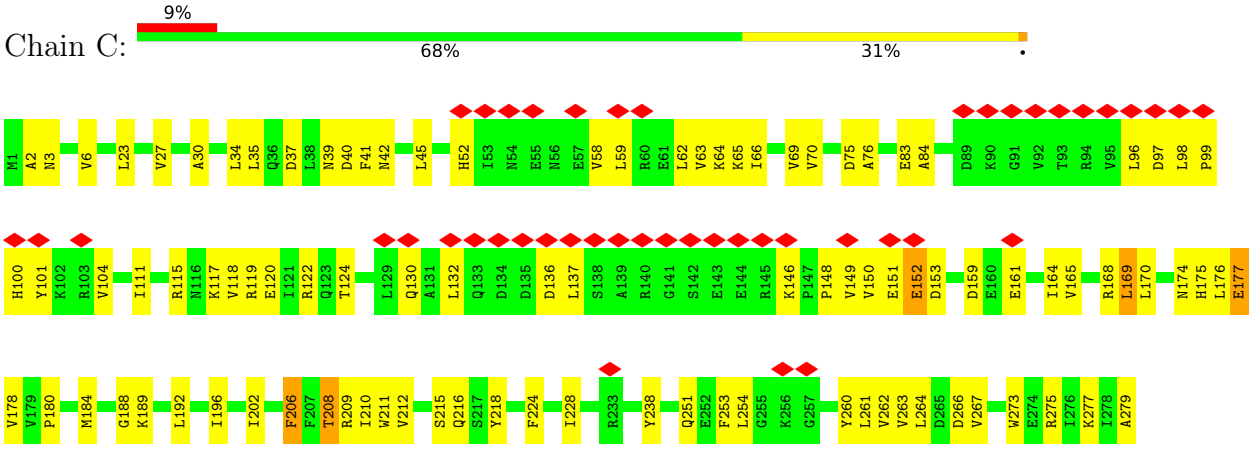
- Molecule 1: NRC2

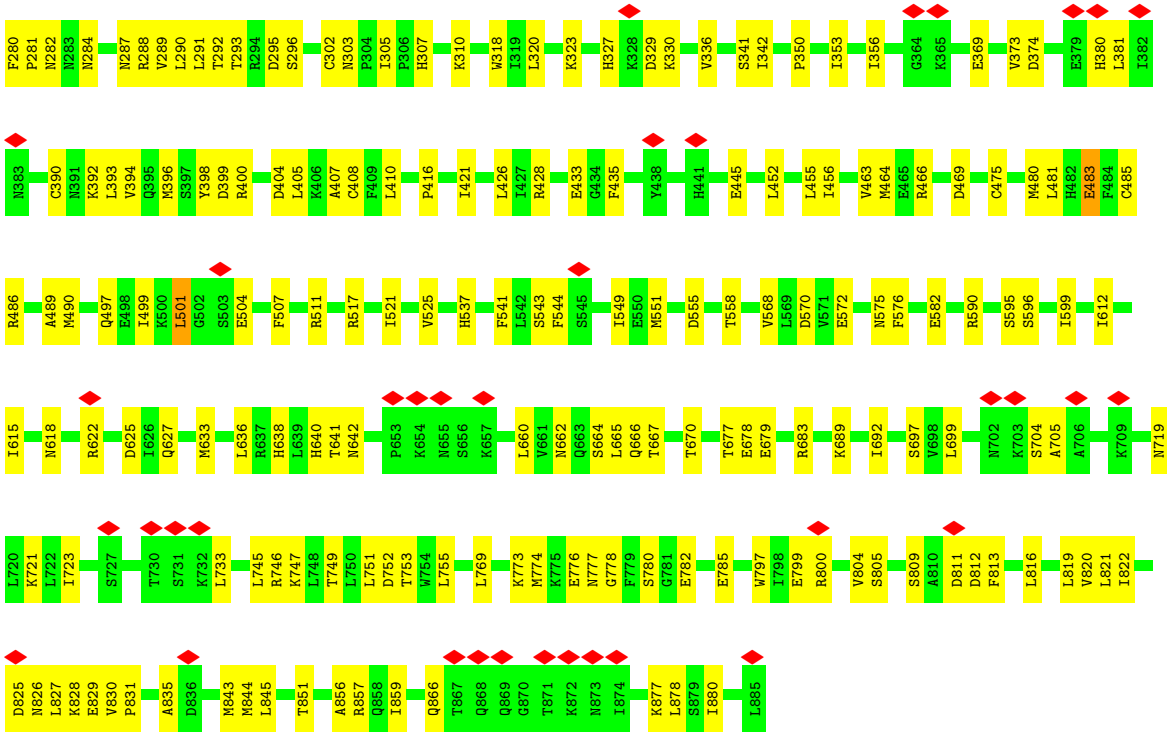
Chain B:



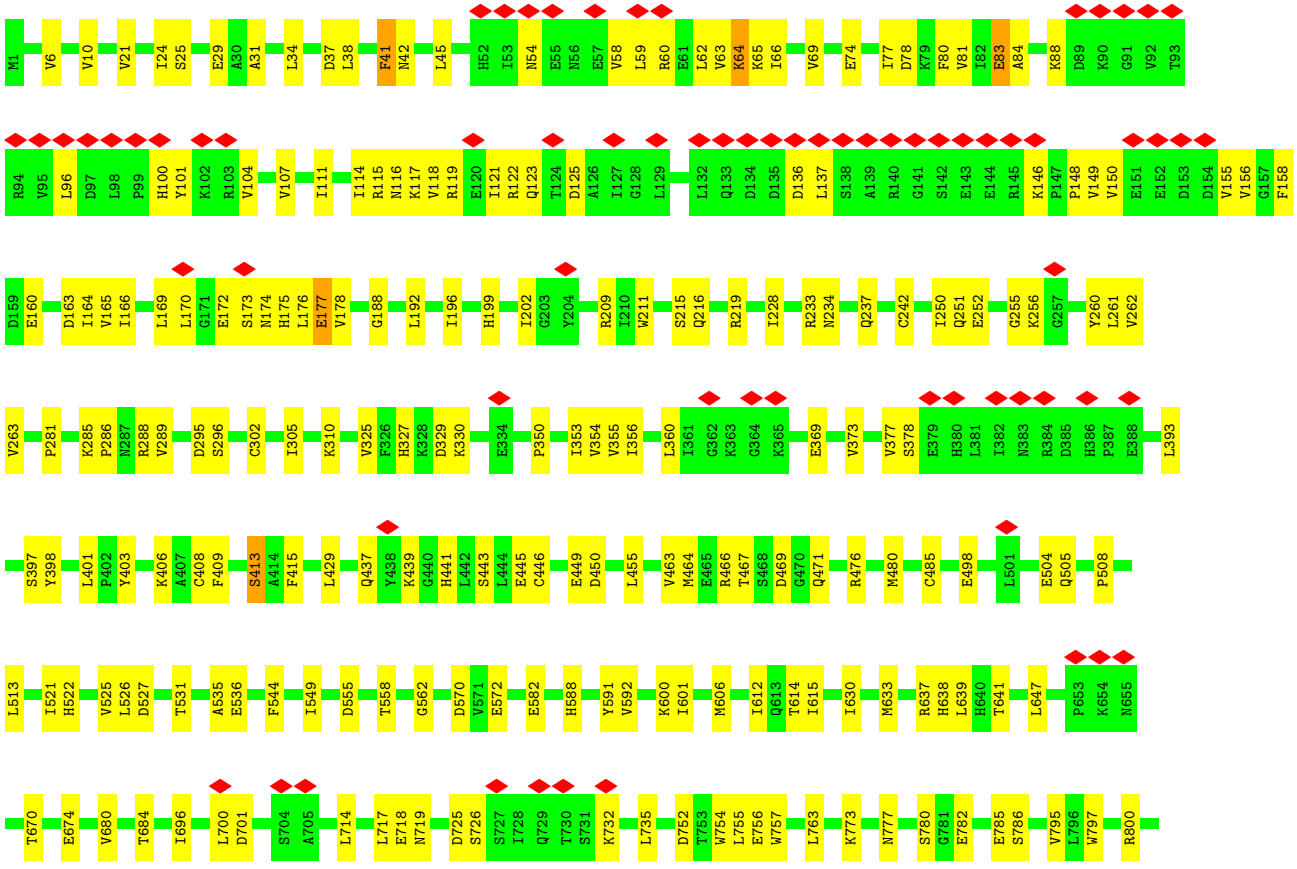
• Molecule 1: NRC2

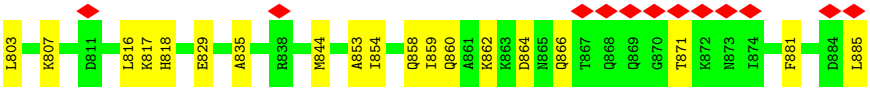
Chain C:



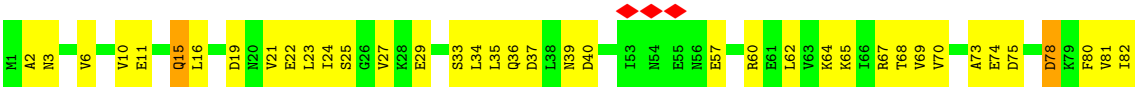


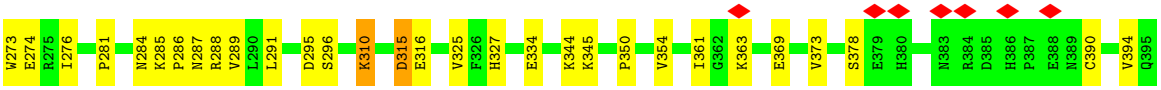
• Molecule 1: NRC2

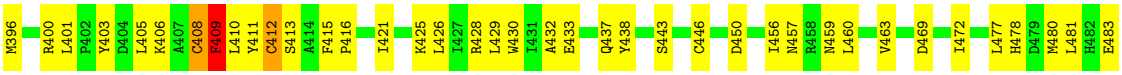


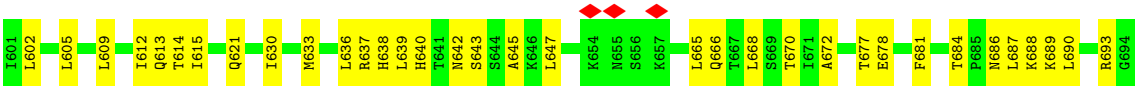


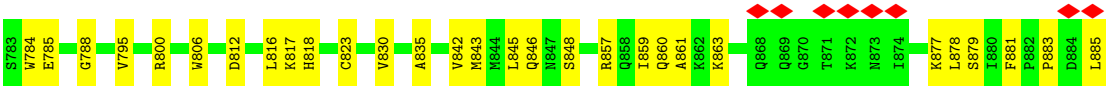
• Molecule 1: NRC2



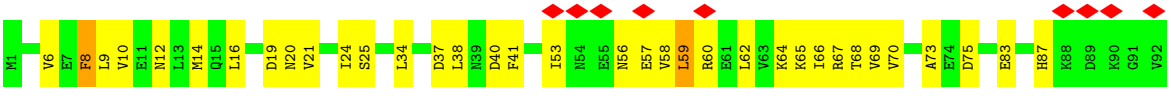


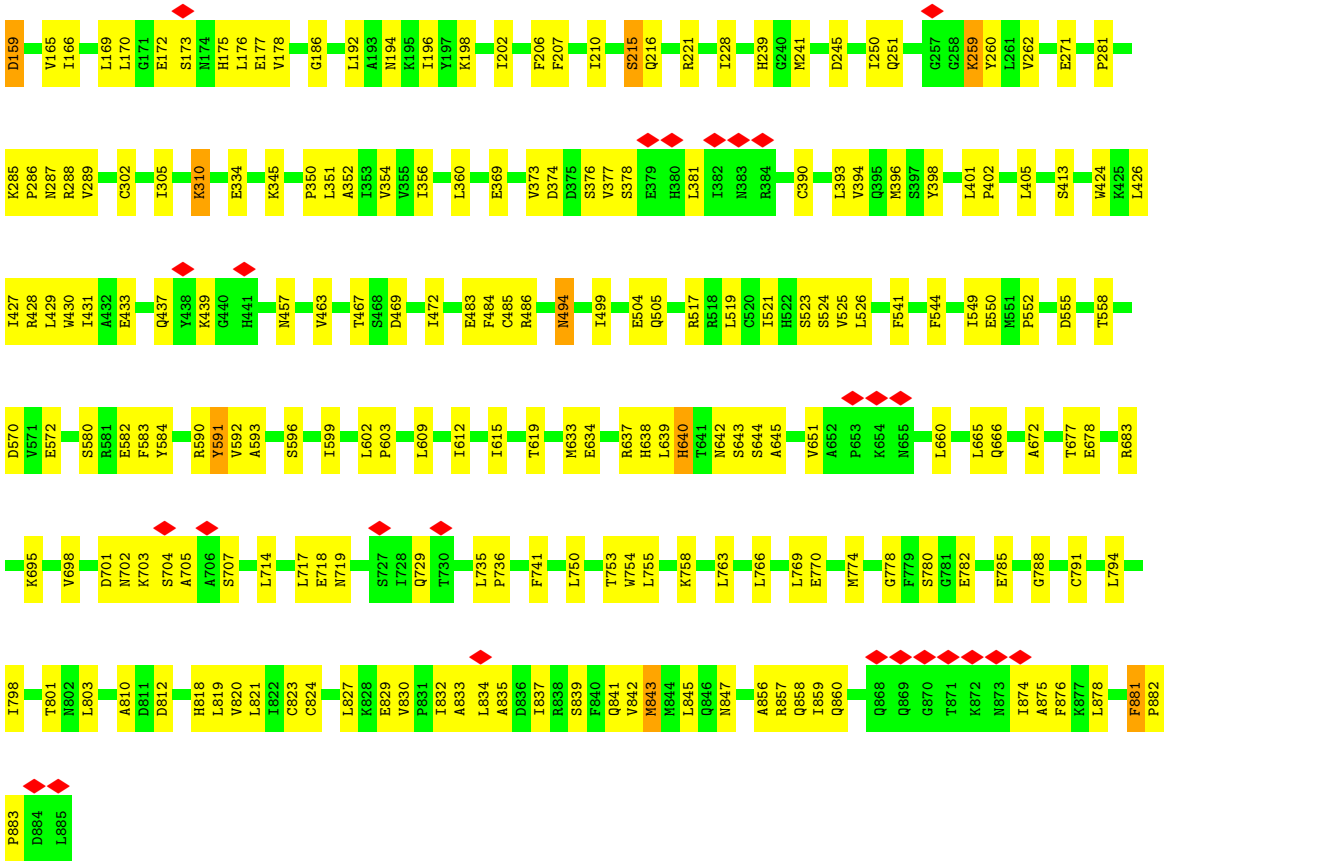






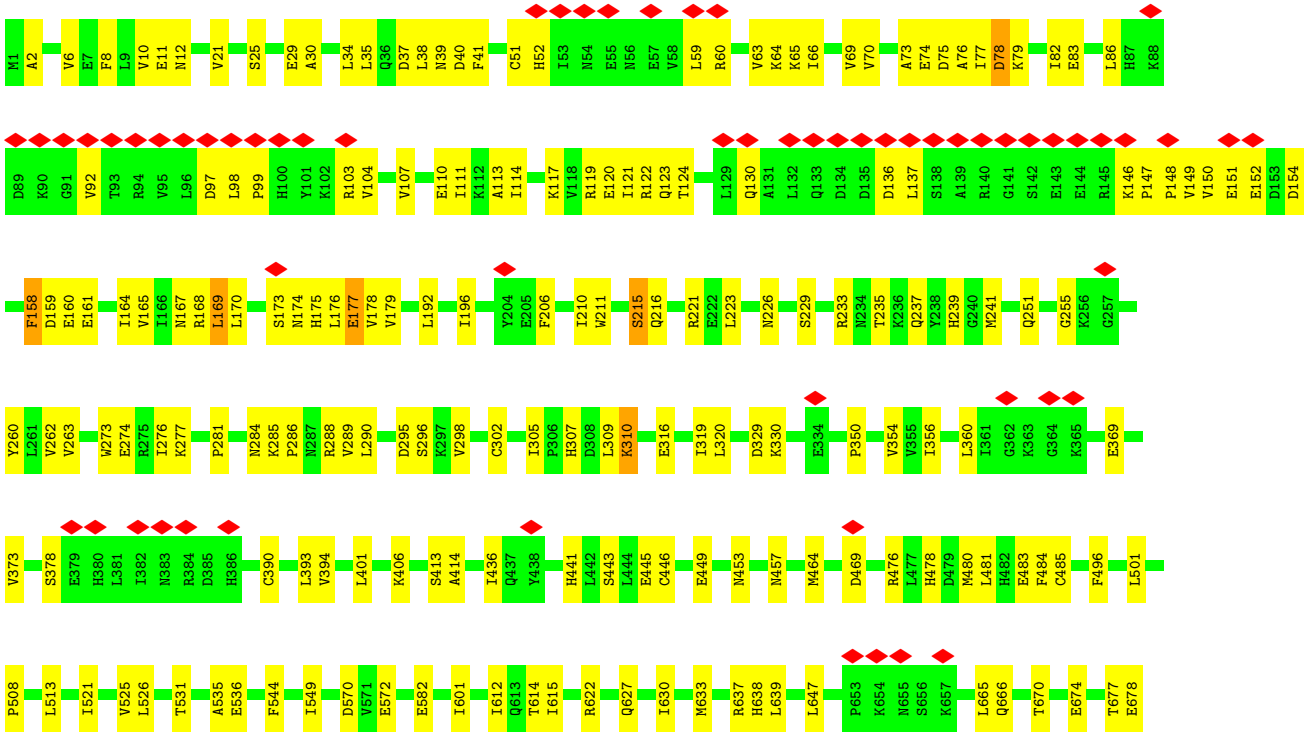
• Molecule 1: NRC2

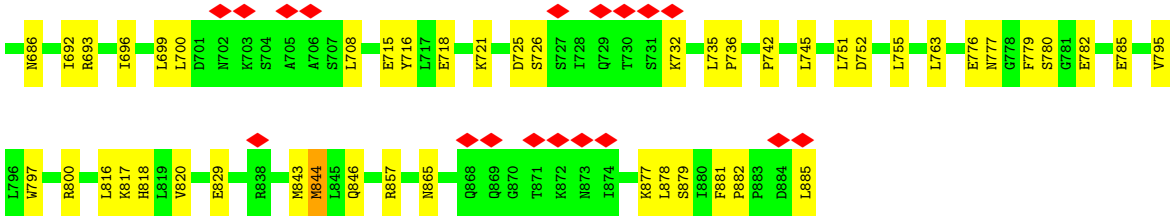




• Molecule 1: NRC2

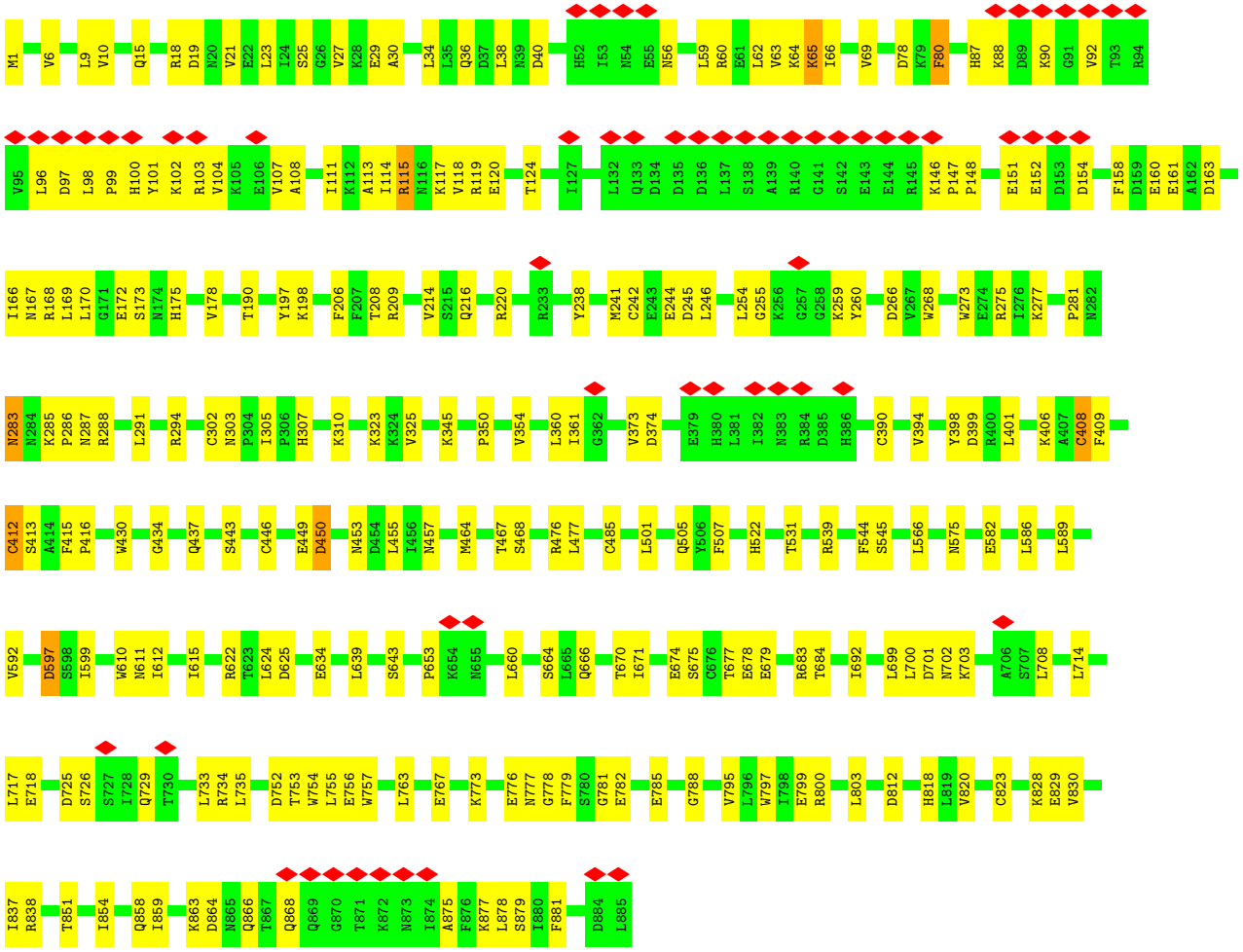
Chain G:





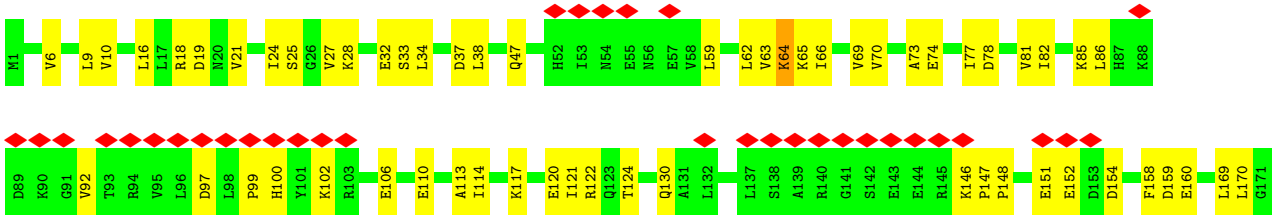
• Molecule 1: NRC2

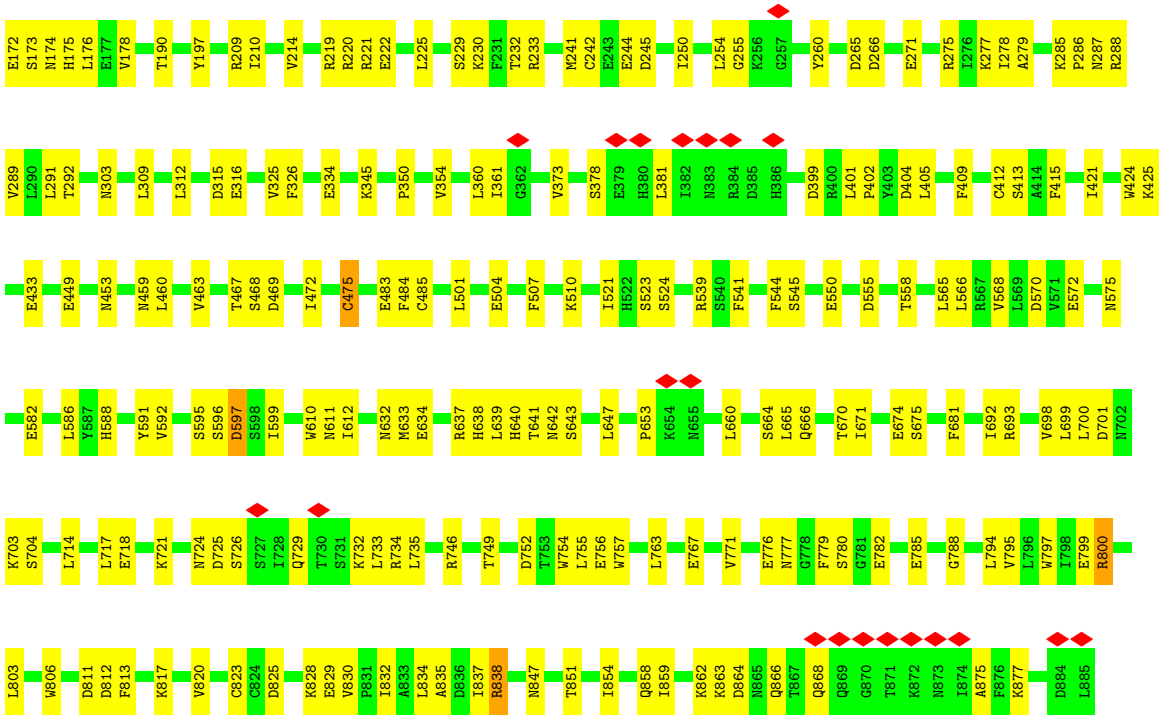
Chain H:



• Molecule 1: NRC2

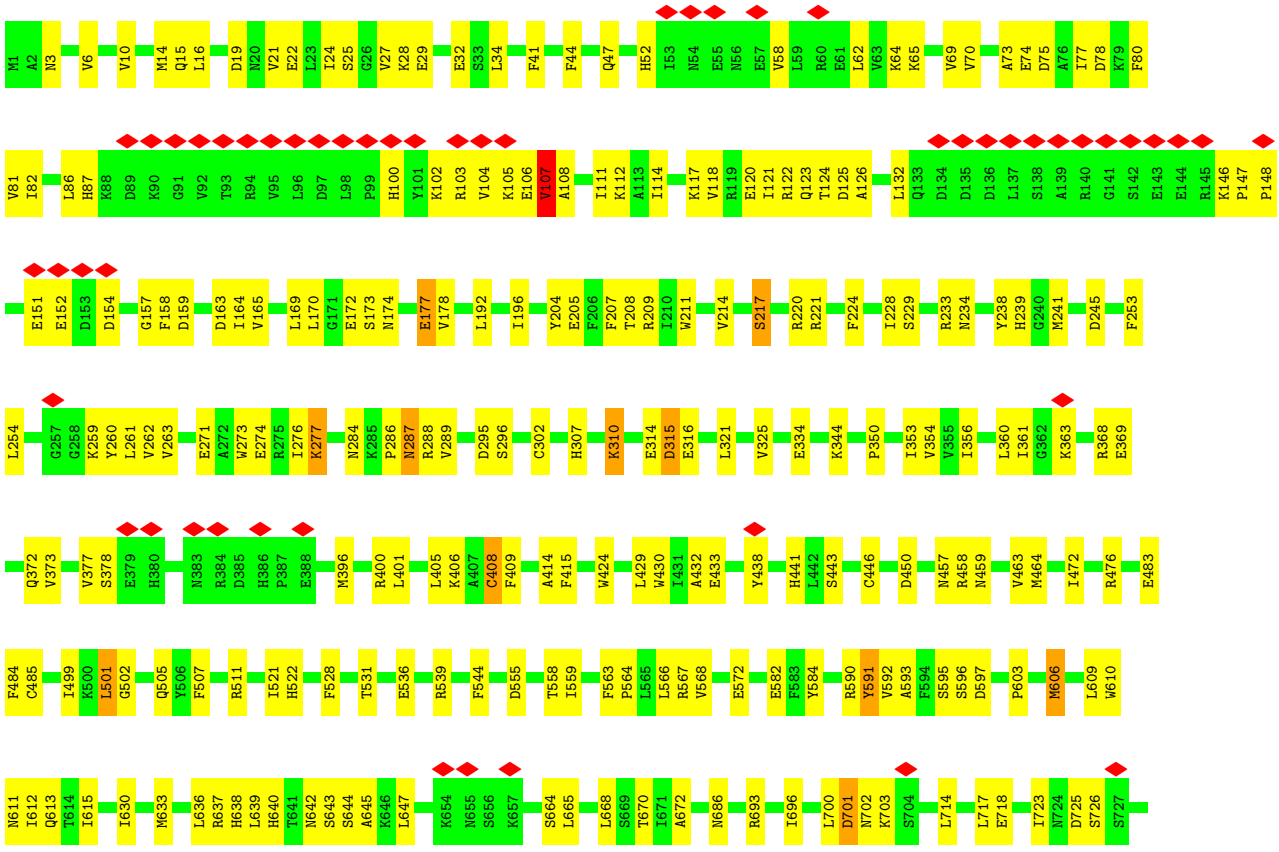
Chain I:

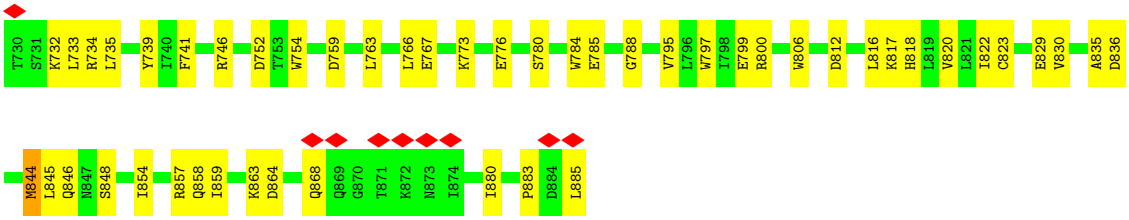




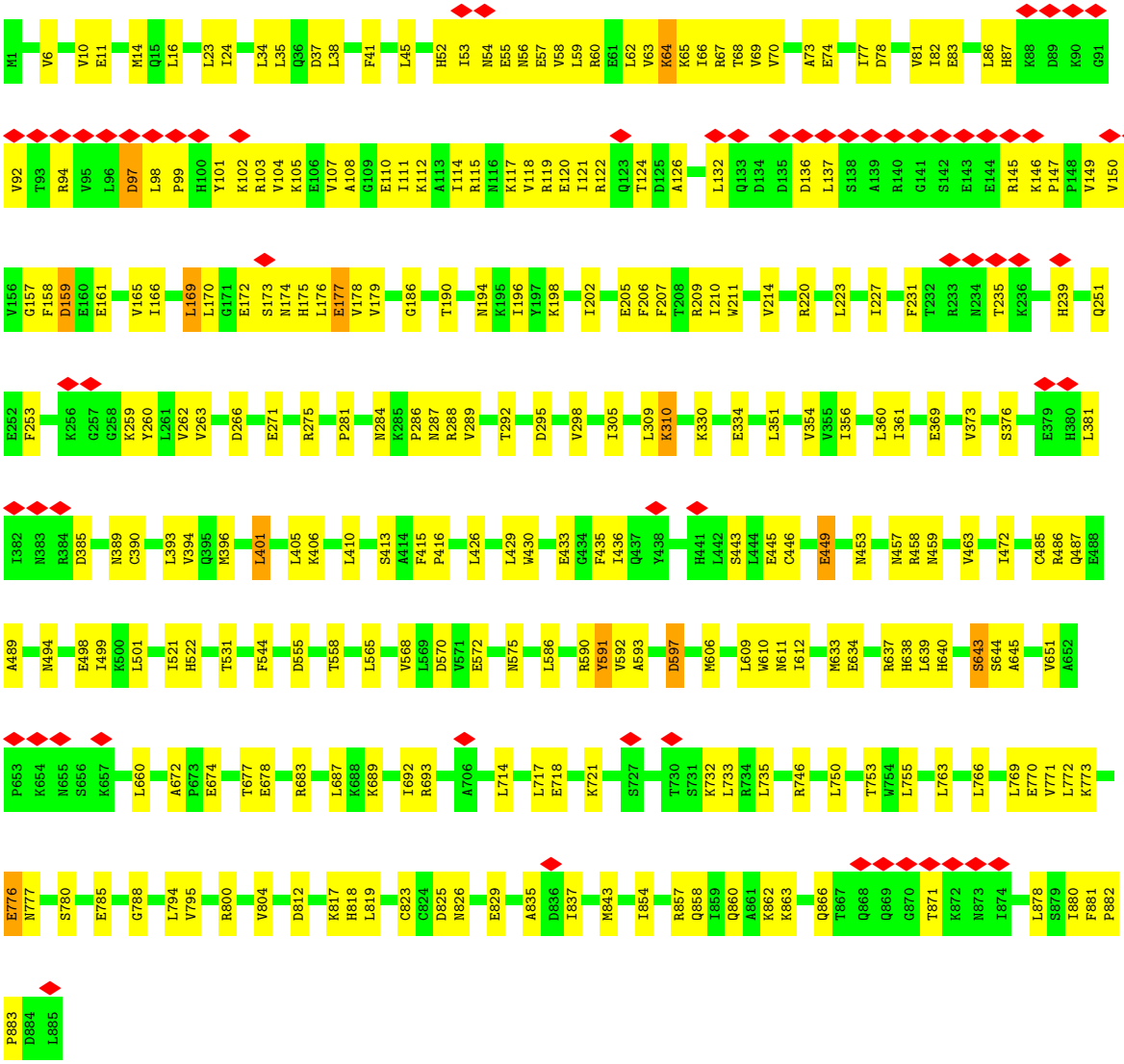
- Molecule 1: NRC2

Chain J:

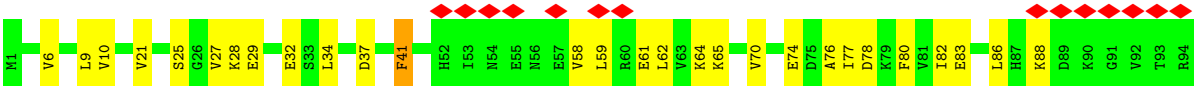


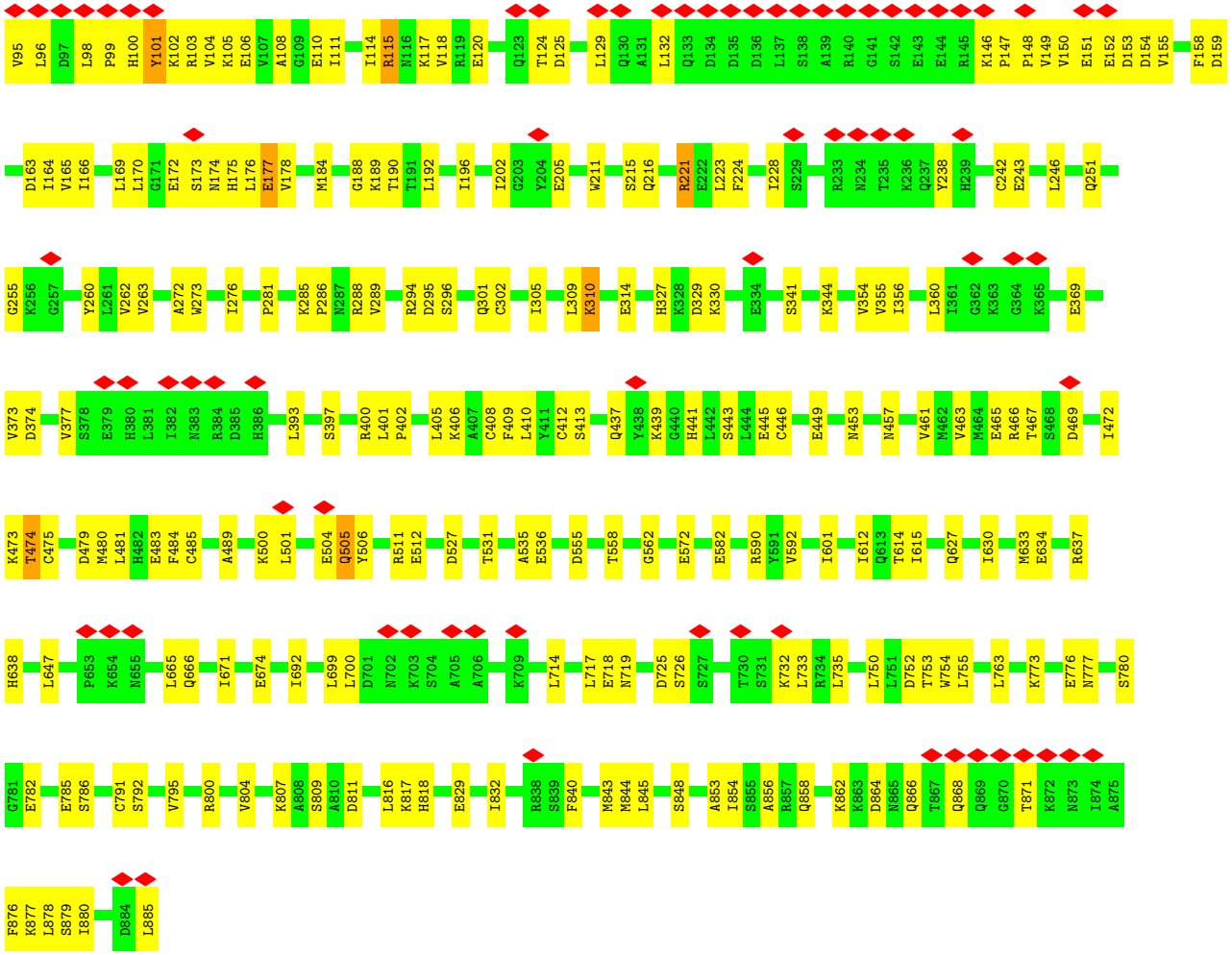


• Molecule 1: NRC2



• Molecule 1: NRC2




V95 L96 D97 L98 P99 H100 Y101 K102 R103 V104 K105 E106 V107 A108 G109 E110 I111 I114 R115 N116 K117 V118 R119 E120 Q123 T124 D125 L129 Q130 A131 L132 Q133 D134 D135 D136 L137 S138 A139 R140 G141 S142 E143 E144 R145 K146 P147 P148 V149 V150 E151 E152 D153 D154 V155 F158 D159
D163 I164 V165 I166 L169 L170 G171 E172 S173 N174 H175 L176 E177 V178 M184 G188 K189 T190 T191 L192 I196 I202 G203 Y204 E205 W211 S215 Q216 R221 E222 L223 F224 I228 S229 R233 N234 T235 K236 Q237 Y238 H239 C242 E243 L246 Q251
G255 K256 G257 Y260 L261 V262 V263 A272 W273 I276 P281 K285 P286 N287 R288 V289 R294 D295 S296 Q301 C302 I305 L309 K310 E314 H327 K328 D329 K330 E334 S341 K344 V354 V355 I356 L360 I361 G362 K363 G364 K365 E369
V373 D374 V377 S378 E379 H380 L381 I382 N383 R384 D385 H386 L393 S397 R400 L401 P402 L405 K406 A407 C408 F409 L410 Y411 C412 S413 Q437 Y438 K439 G440 H441 L442 S443 L444 E445 C446 E449 N453 M457 V461 M462 V463 M464 E465 R466 T467 S468 D469 I472
K473 T474 C475 D479 M480 L481 H482 E483 F484 C485 A489 K500 L501 E504 Q505 Y506 R511 E512 D527 T531 A535 E536 D555 T558 G562 E572 E582 R590 Y591 V592 I601 I612 Q613 T614 I615 Q627 I630 M633 E634 R637
H638 L647 P653 K654 N655 L665 Q666 I671 E674 I692 L699 L700 D701 N702 K703 S704 A705 A706 K709 L714 L717 E718 N719 D725 S726 S727 T730 S731 K732 L733 R734 L735 L750 L751 D752 T753 W754 L755 L763 K773 E776 N777 S780
G781 E782 E785 S786 C791 S792 V795 R800 V804 K807 A808 S809 A810 D811 L816 K817 H818 E829 I832 R838 S839 F840 M843 M844 L845 S848 A853 I854 S855 A856 R857 Q858 K862 K863 D864 N865 Q866 T867 Q868 Q869 G870 T871 K872 N873 I874 A875
F876 K877 L878 S879 I880 D884 L886

4 Experimental information (i)

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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	17.142	Depositor
Minimum map value	-10.408	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	281.0624, 281.0624, 281.0624	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

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

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:H1'	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%)	51	83
1	D	883/885 (100%)	835 (95%)	48 (5%)	0	100	100
1	E	883/885 (100%)	806 (91%)	74 (8%)	3 (0%)	41	75
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%)	51	83
1	I	883/885 (100%)	824 (93%)	59 (7%)	0	100	100
1	J	883/885 (100%)	804 (91%)	78 (9%)	1 (0%)	51	83
1	K	883/885 (100%)	821 (93%)	61 (7%)	1 (0%)	51	83
1	L	883/885 (100%)	836 (95%)	47 (5%)	0	100	100
All	All	10596/10620 (100%)	9893 (93%)	696 (7%)	7 (0%)	54	83

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%)	57	80
1	B	797/797 (100%)	779 (98%)	18 (2%)	50	76
1	C	797/797 (100%)	773 (97%)	24 (3%)	41	71
1	D	797/797 (100%)	783 (98%)	14 (2%)	59	81
1	E	797/797 (100%)	767 (96%)	30 (4%)	33	66
1	F	797/797 (100%)	780 (98%)	17 (2%)	53	78
1	G	797/797 (100%)	781 (98%)	16 (2%)	55	79
1	H	797/797 (100%)	780 (98%)	17 (2%)	53	78
1	I	797/797 (100%)	783 (98%)	14 (2%)	59	81
1	J	797/797 (100%)	768 (96%)	29 (4%)	35	67
1	K	797/797 (100%)	778 (98%)	19 (2%)	49	75
1	L	797/797 (100%)	782 (98%)	15 (2%)	57	80
All	All	9564/9564 (100%)	9336 (98%)	228 (2%)	51	75

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	C	901	-	36,36,36	1.48	6 (16%)	54,60,60	0.57	0
3	ADP	E	902	-	24,29,29	0.71	0	29,45,45	0.70	1 (3%)
2	IHP	L	901	-	36,36,36	1.43	6 (16%)	54,60,60	0.64	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	IHP	G	901	-	36,36,36	0.75	0	54,60,60	0.61	0
3	ADP	C	902	-	24,29,29	0.95	1 (4%)	29,45,45	1.41	4 (13%)
3	ADP	J	902	-	24,29,29	0.73	0	29,45,45	0.78	0
2	IHP	J	901	-	36,36,36	0.74	0	54,60,60	0.54	0
2	IHP	E	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.65	1 (1%)
3	ADP	F	902	-	24,29,29	0.70	1 (4%)	29,45,45	0.79	1 (3%)
3	ADP	A	902	-	24,29,29	0.79	0	29,45,45	0.79	1 (3%)
2	IHP	D	901	-	36,36,36	0.76	0	54,60,60	0.56	0
2	IHP	B	901	-	36,36,36	0.76	0	54,60,60	0.60	0
3	ADP	D	902	-	24,29,29	0.71	0	29,45,45	0.85	1 (3%)
3	ADP	B	902	-	24,29,29	0.72	0	29,45,45	0.78	1 (3%)
3	ADP	L	902	-	24,29,29	0.70	0	29,45,45	0.88	0
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%)
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	K	901	-	36,36,36	1.44	6 (16%)	54,60,60	0.61	0
2	IHP	H	901	-	36,36,36	1.45	6 (16%)	54,60,60	0.73	2 (3%)
3	ADP	K	902	-	24,29,29	0.67	0	29,45,45	0.92	2 (6%)
3	ADP	G	902	-	24,29,29	0.69	0	29,45,45	0.92	2 (6%)
2	IHP	F	901	-	36,36,36	0.73	0	54,60,60	0.56	0

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	C	901	-	-	7/30/54/54	0/1/1/1
3	ADP	E	902	-	-	6/12/32/32	0/3/3/3
2	IHP	L	901	-	-	14/30/54/54	0/1/1/1
2	IHP	G	901	-	-	13/30/54/54	0/1/1/1
3	ADP	C	902	-	-	5/12/32/32	0/3/3/3
3	ADP	J	902	-	-	1/12/32/32	0/3/3/3
2	IHP	J	901	-	-	7/30/54/54	0/1/1/1
2	IHP	E	901	-	-	18/30/54/54	0/1/1/1
3	ADP	F	902	-	-	9/12/32/32	0/3/3/3
3	ADP	A	902	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IHP	D	901	-	-	8/30/54/54	0/1/1/1
2	IHP	B	901	-	-	15/30/54/54	0/1/1/1
3	ADP	D	902	-	-	5/12/32/32	0/3/3/3
3	ADP	B	902	-	-	1/12/32/32	0/3/3/3
3	ADP	L	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
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	K	901	-	-	12/30/54/54	0/1/1/1
2	IHP	H	901	-	-	16/30/54/54	0/1/1/1
3	ADP	K	902	-	-	4/12/32/32	0/3/3/3
3	ADP	G	902	-	-	7/12/32/32	0/3/3/3
2	IHP	F	901	-	-	8/30/54/54	0/1/1/1

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(^{o})	Ideal(^{o})
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
3	E	902	ADP	1	0
2	L	901	IHP	1	0
3	C	902	ADP	3	0
3	J	902	ADP	3	0
3	F	902	ADP	4	0
3	A	902	ADP	5	0
2	D	901	IHP	1	0
3	D	902	ADP	6	0
3	B	902	ADP	4	0
3	L	902	ADP	7	0

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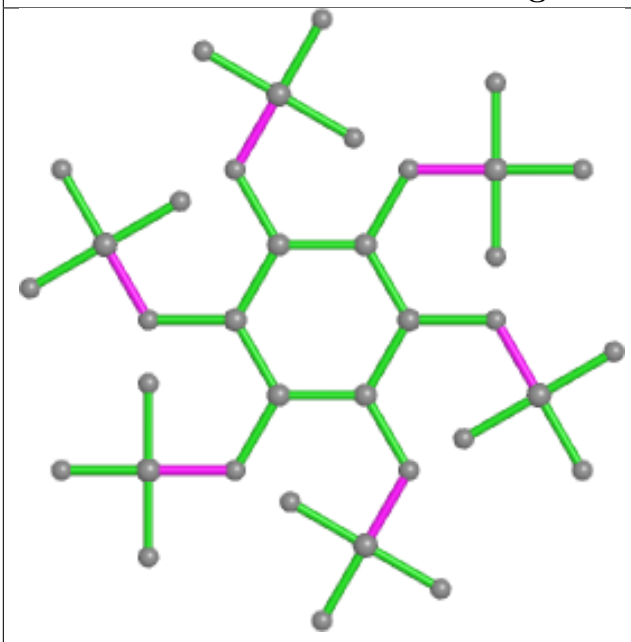
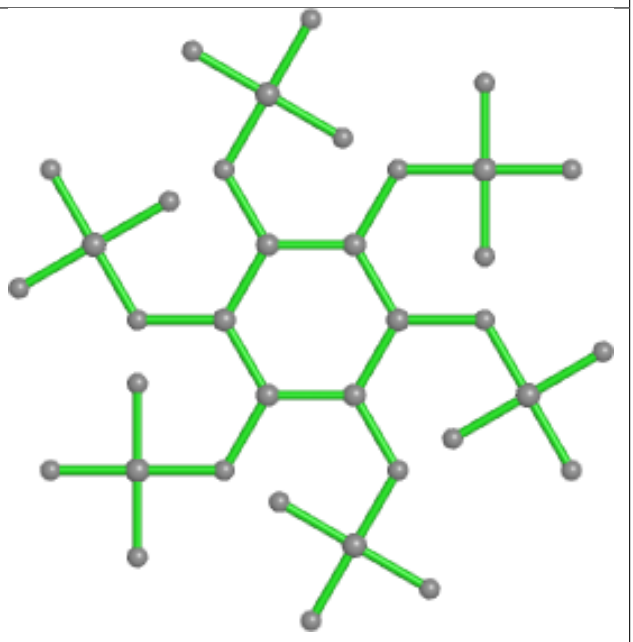
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	902	ADP	3	0
2	I	901	IHP	2	0
3	H	902	ADP	3	0
2	K	901	IHP	1	0
2	H	901	IHP	2	0
3	K	902	ADP	4	0
3	G	902	ADP	1	0

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 then 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.

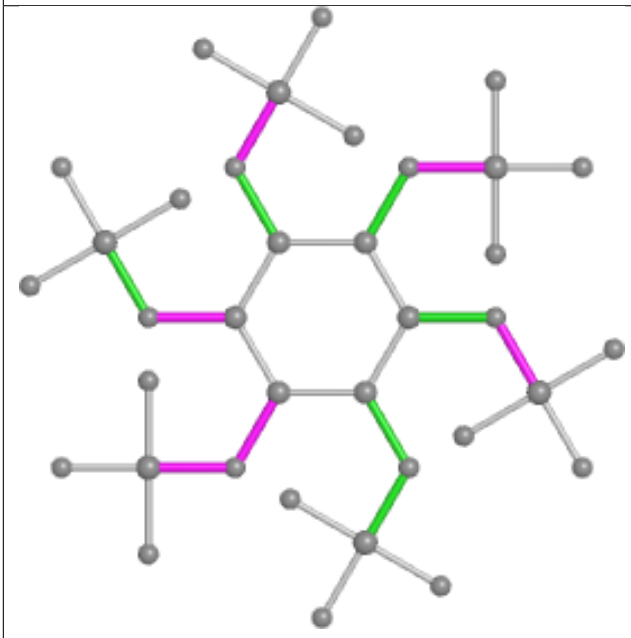
Ligand IHP C 901



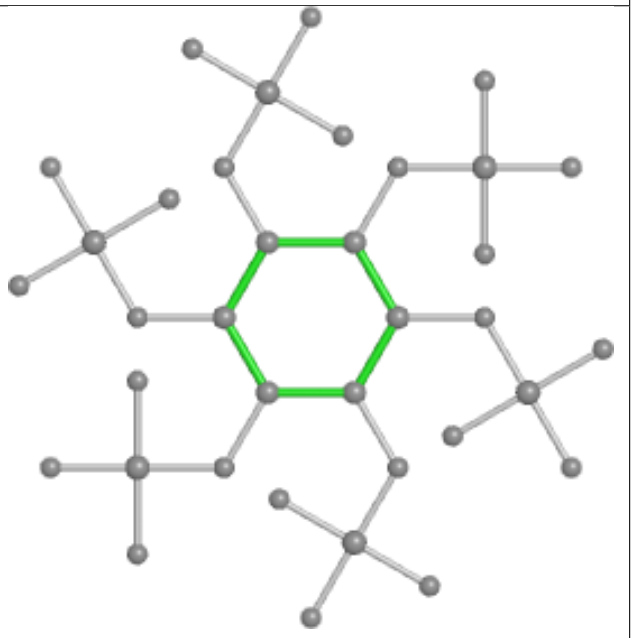
Bond lengths



Bond angles

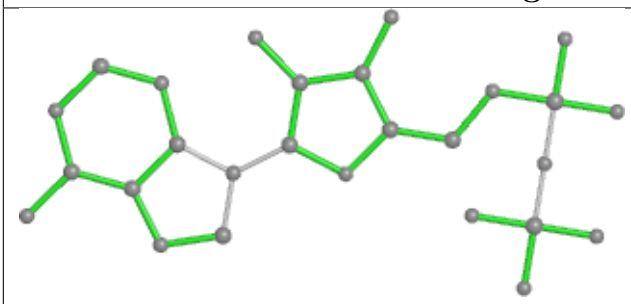


Torsions



Rings

Ligand ADP E 902



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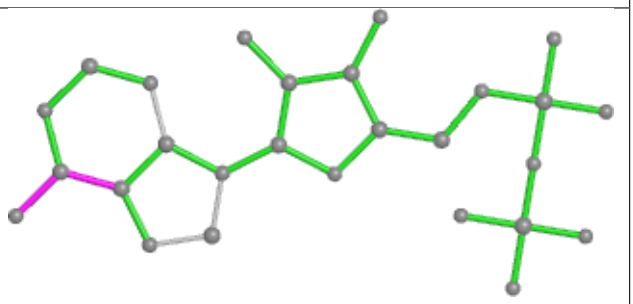

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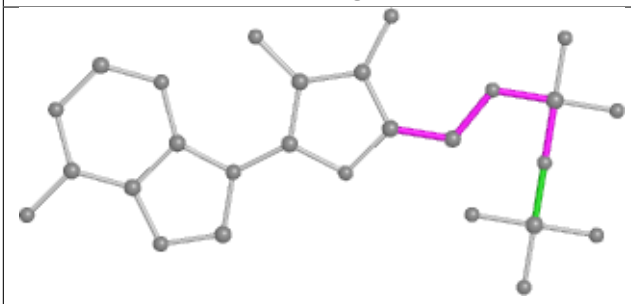

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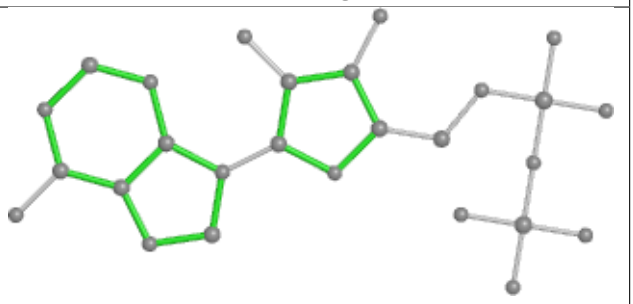
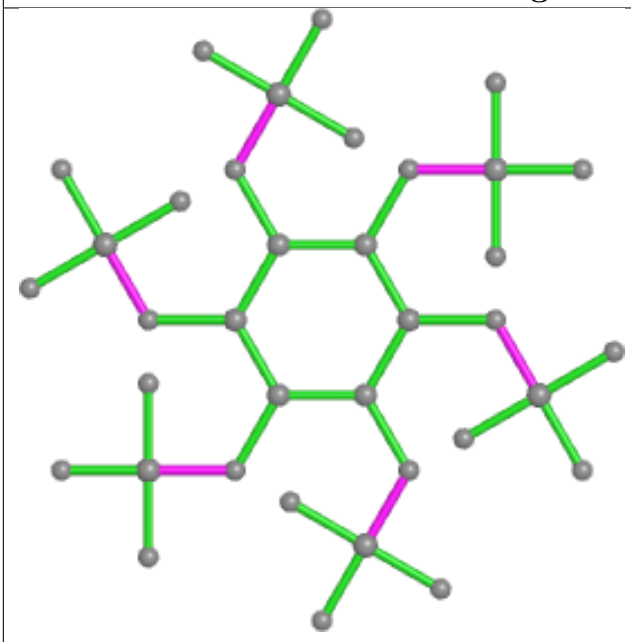


Rings

Ligand IHP L 901



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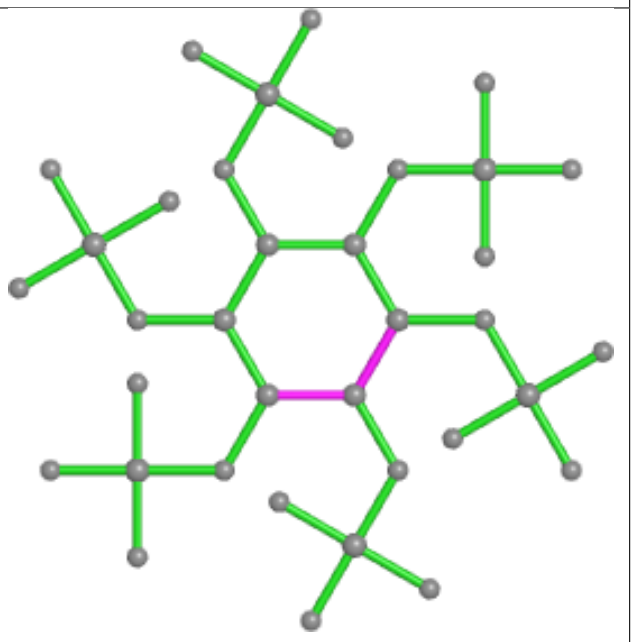
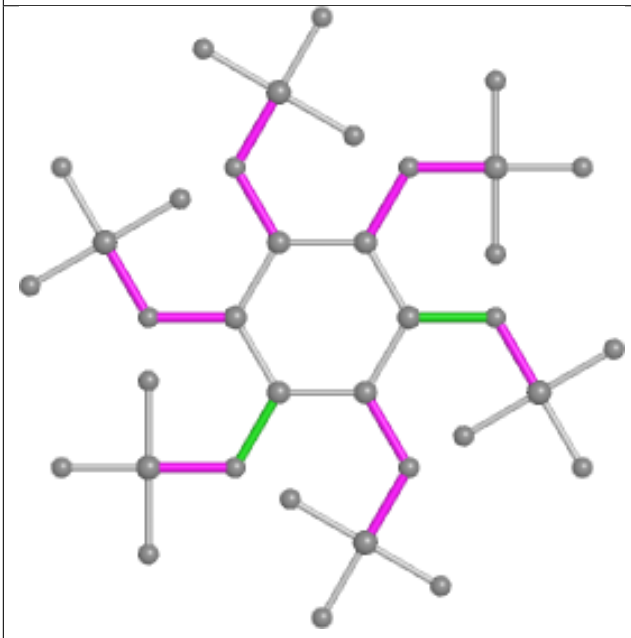
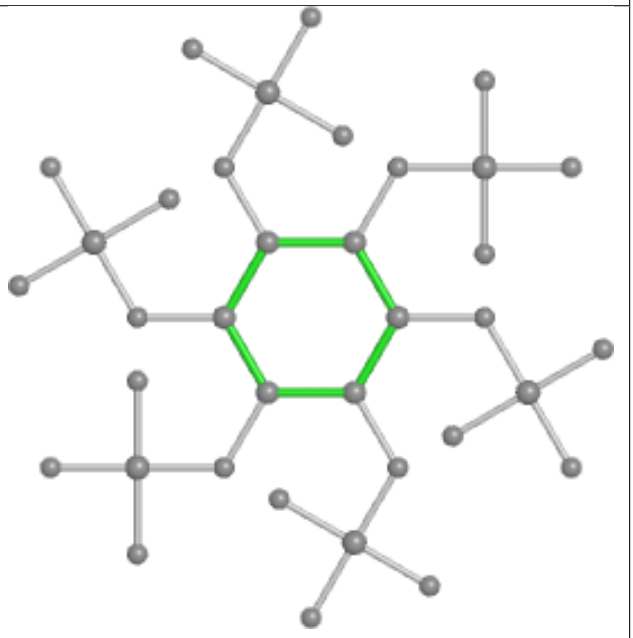


Bond angles

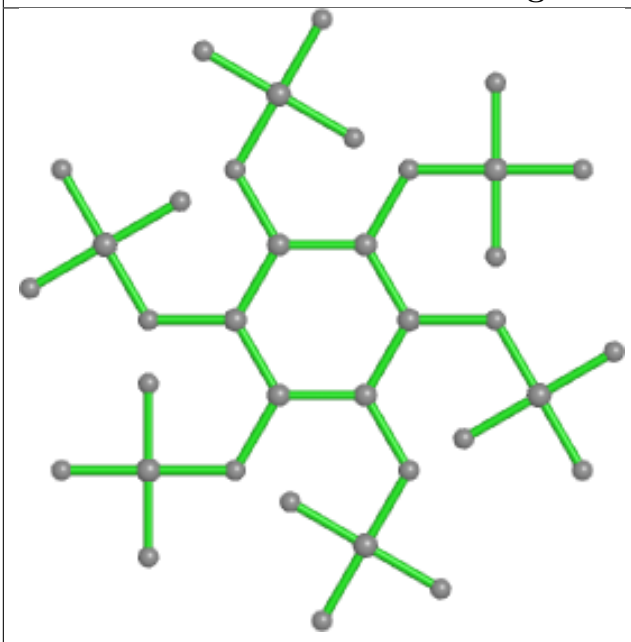


Torsions



Rings

Ligand IHP G 901



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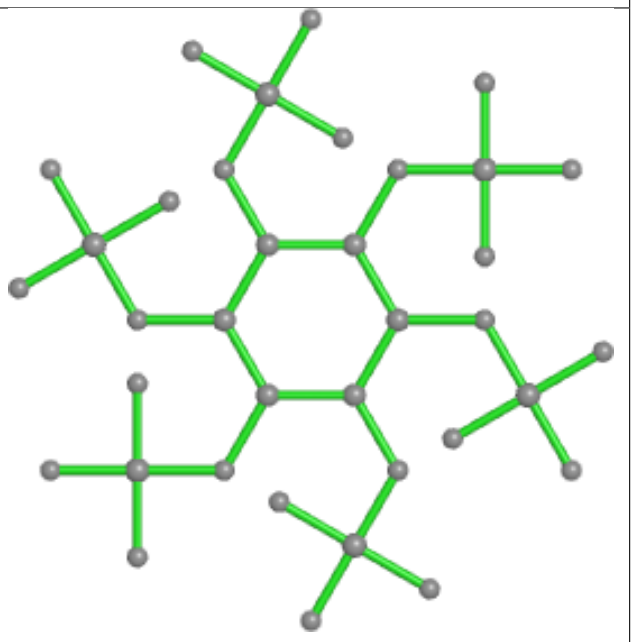

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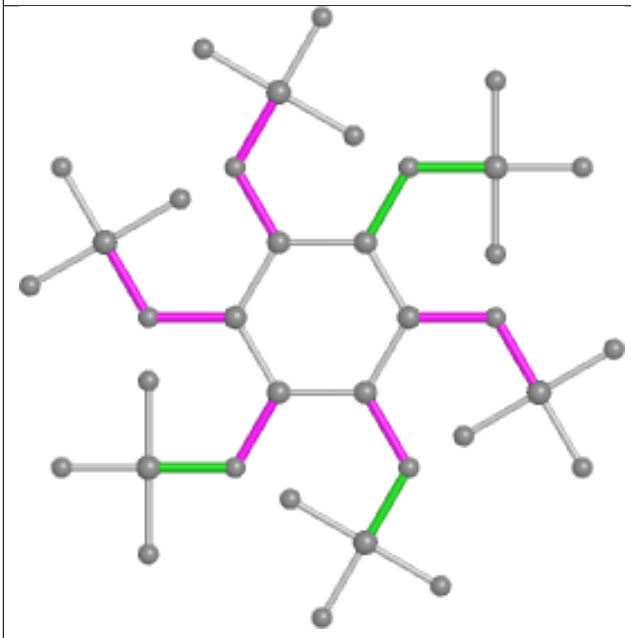

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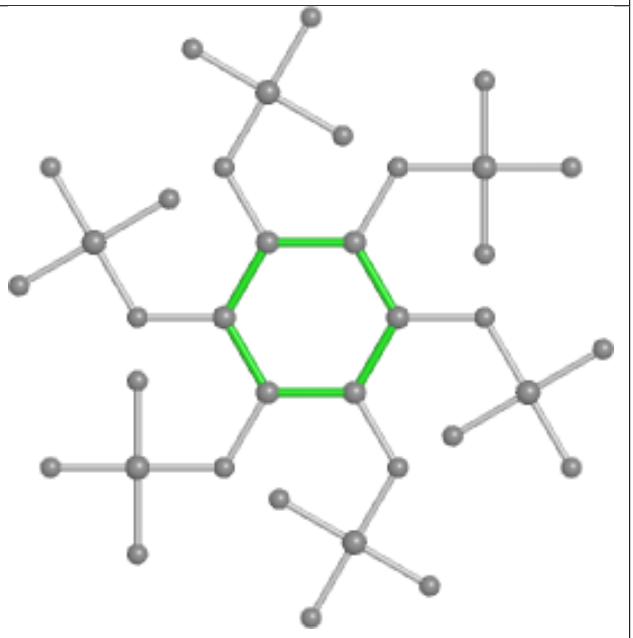
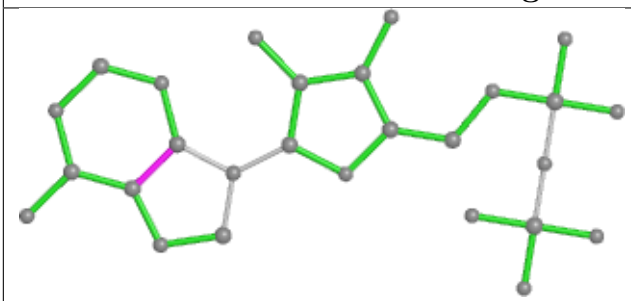


Rings

Ligand ADP C 902



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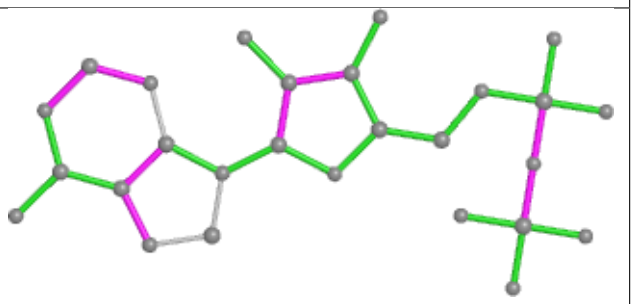

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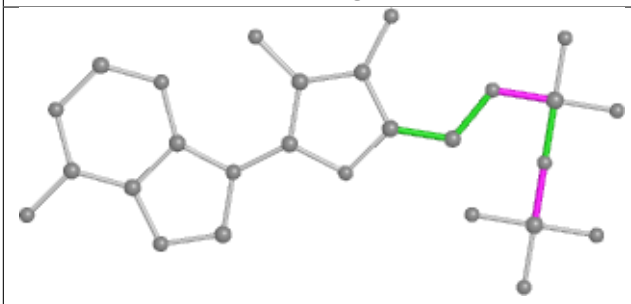

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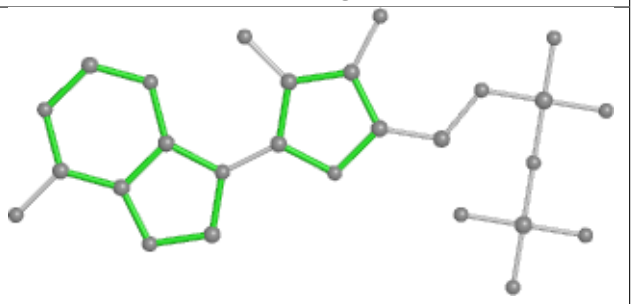
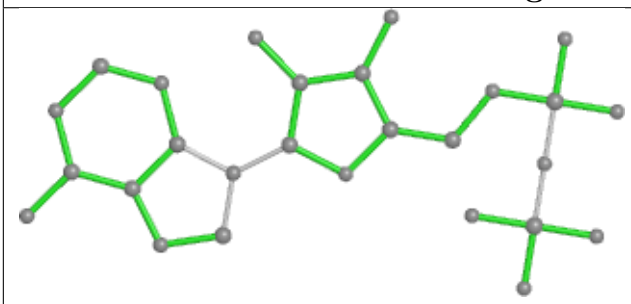


Rings

Ligand ADP J 902



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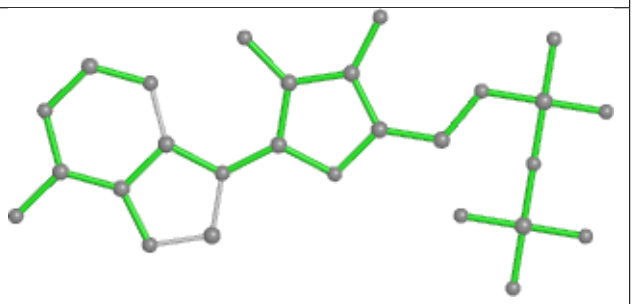

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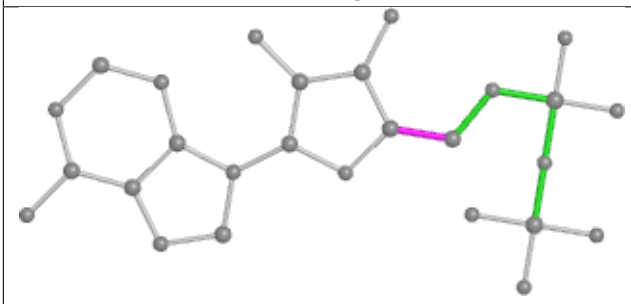

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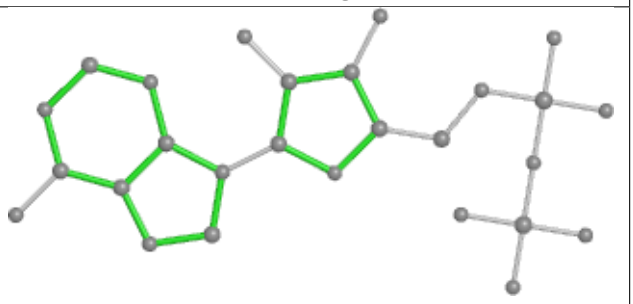
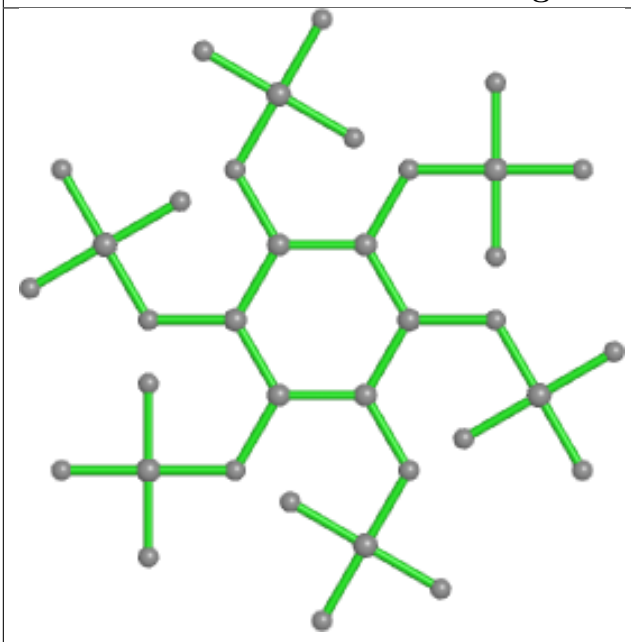


Rings

Ligand IHP J 901



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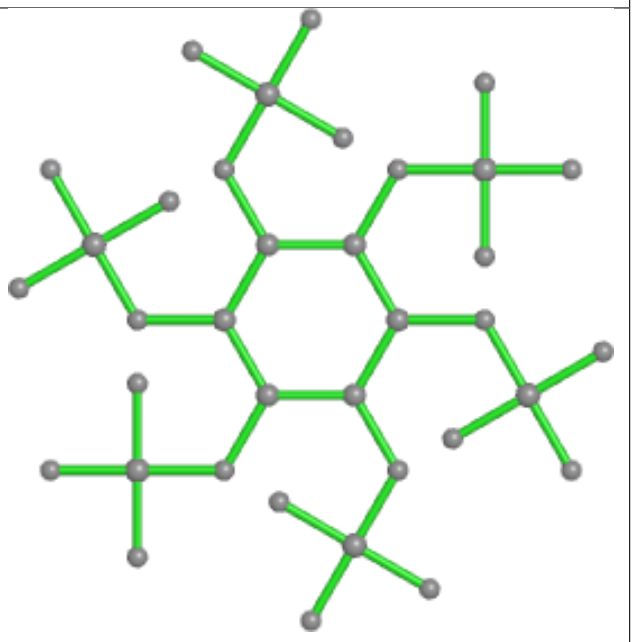

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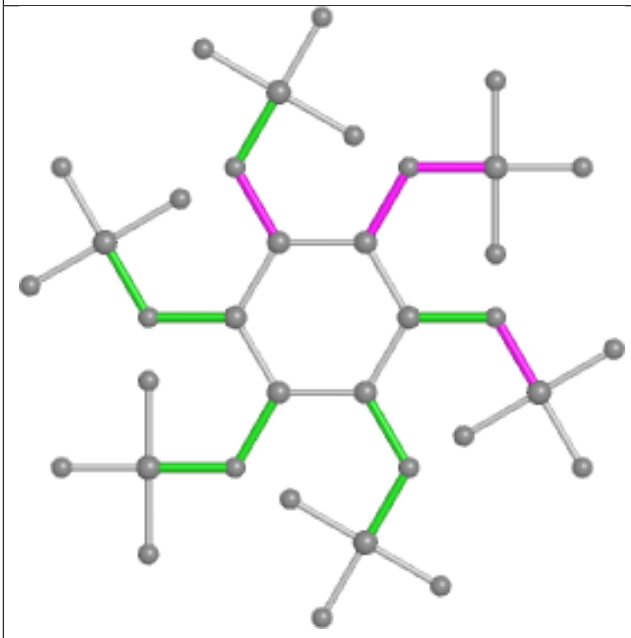

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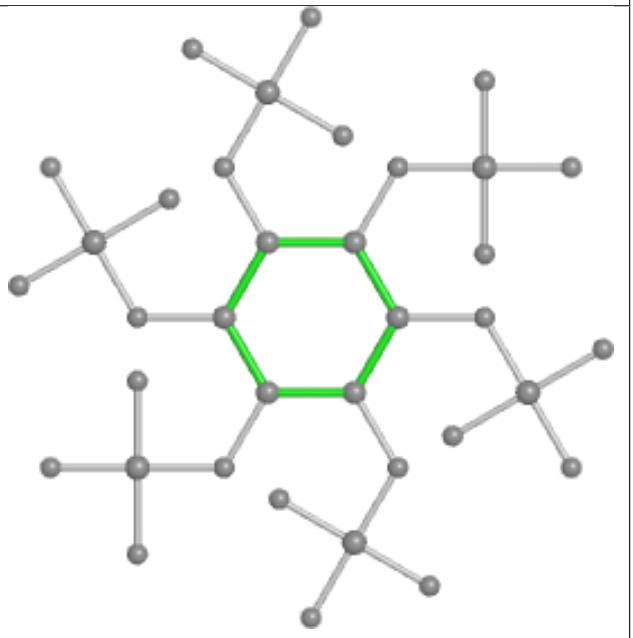
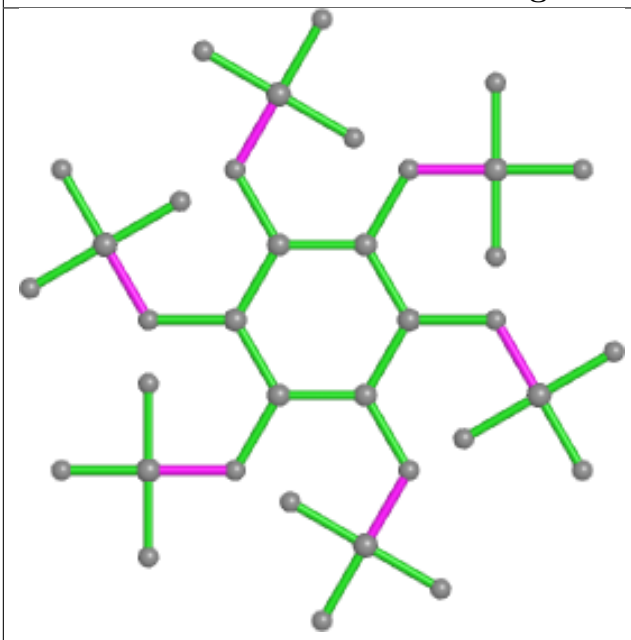


Rings

Ligand IHP E 901



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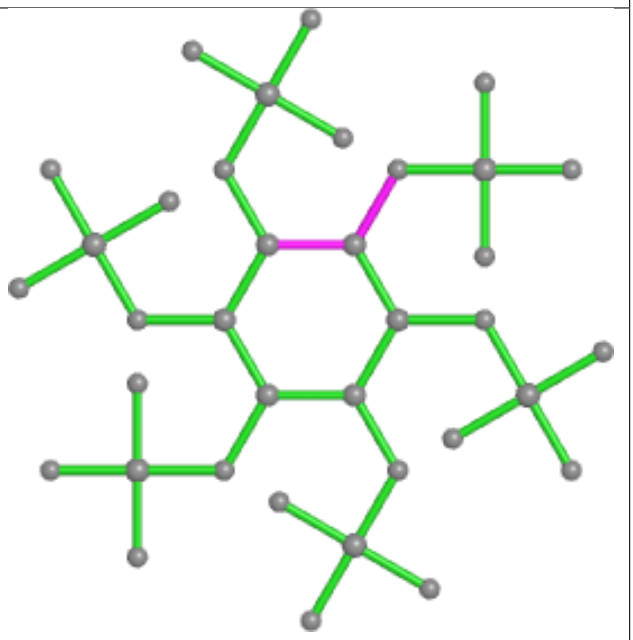

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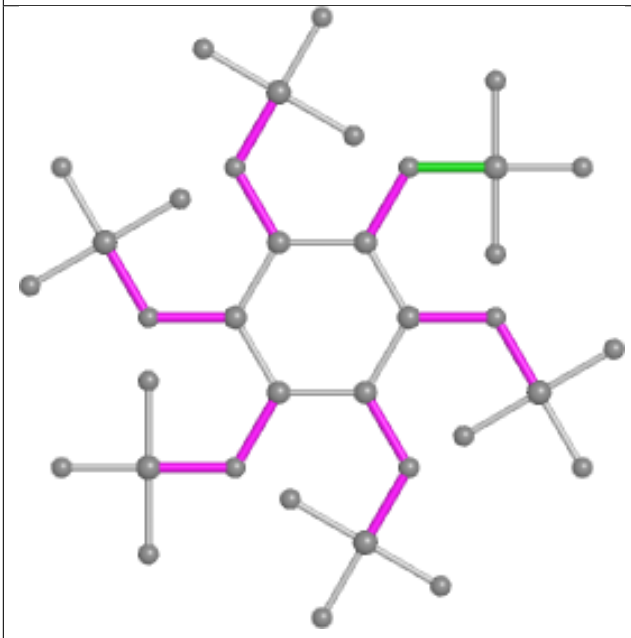

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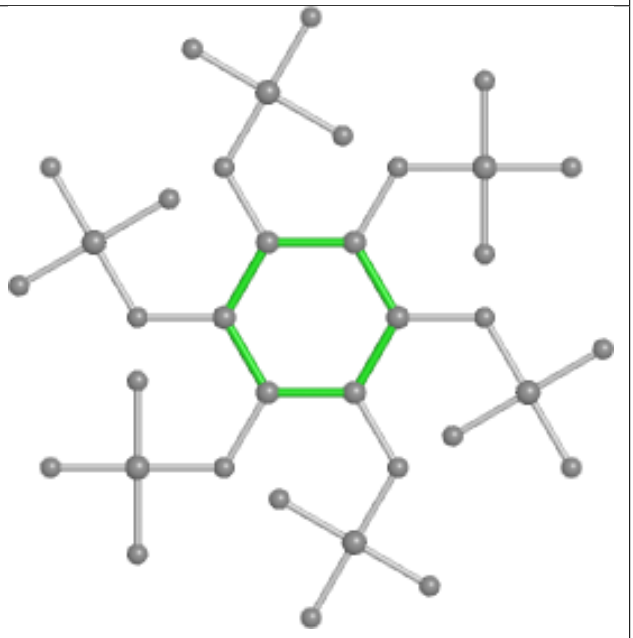
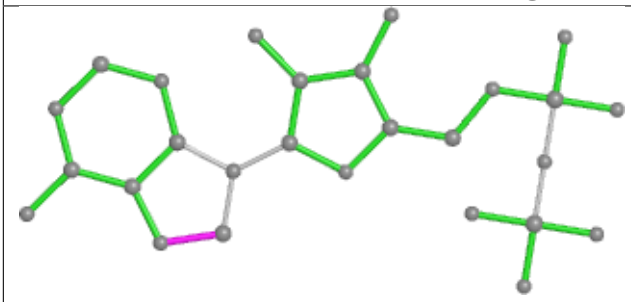
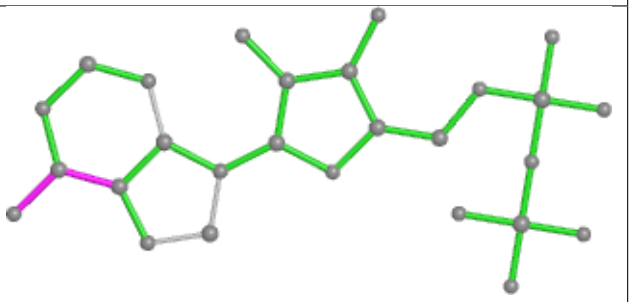
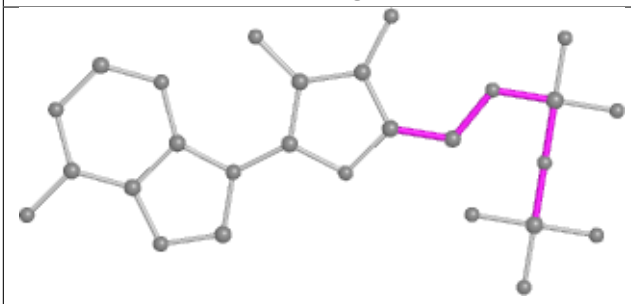
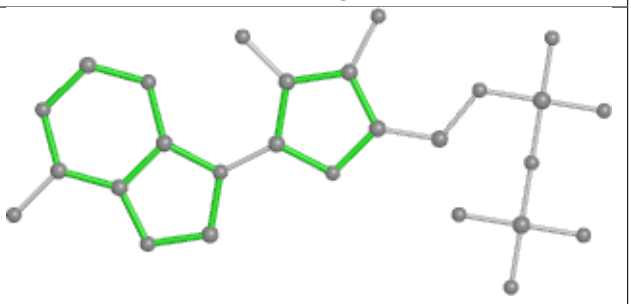
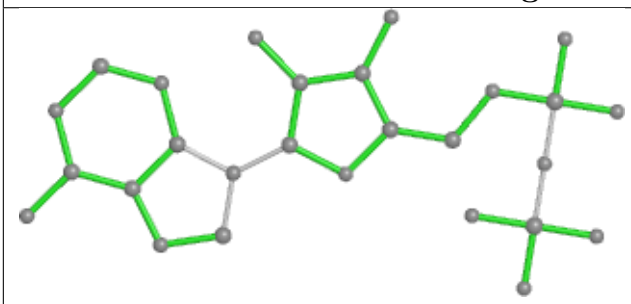
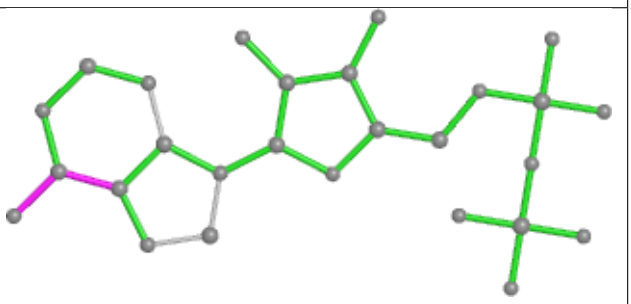
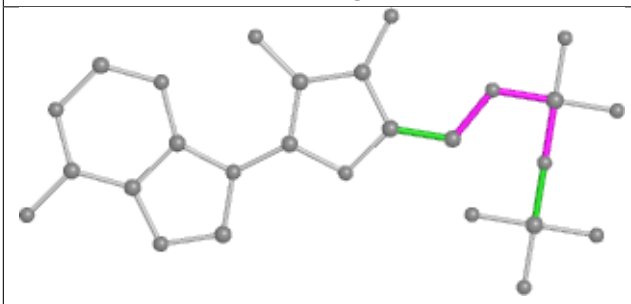
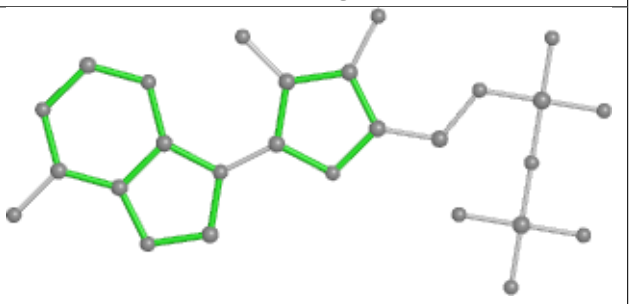
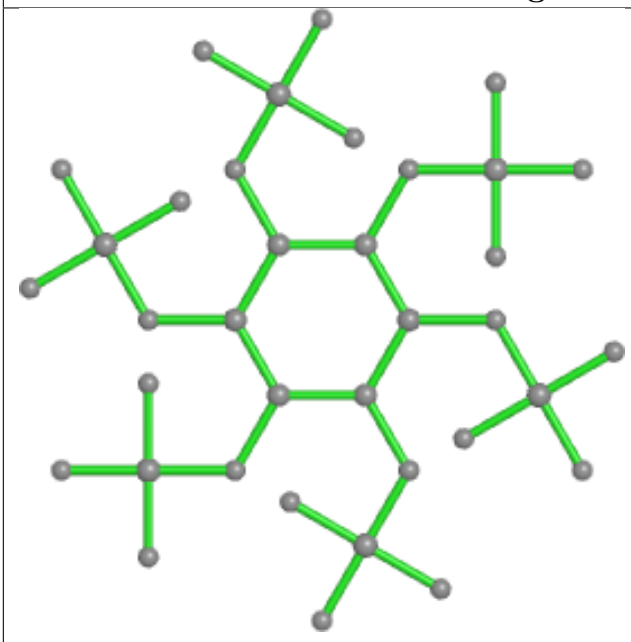


Rings

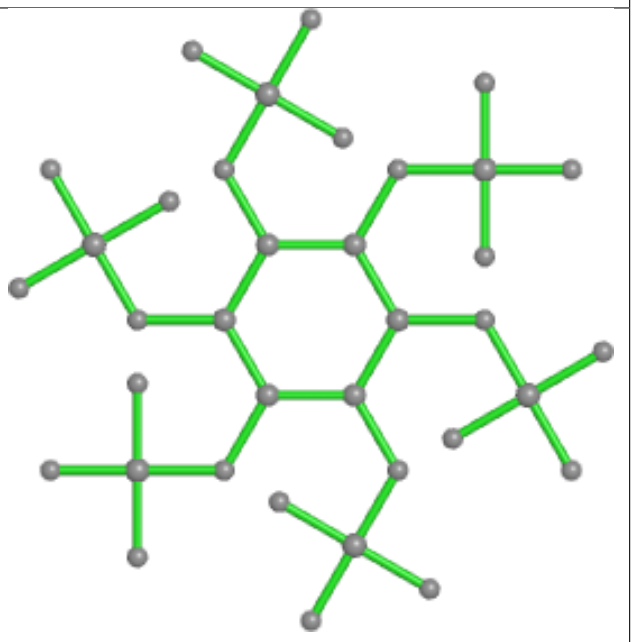
Ligand ADP F 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

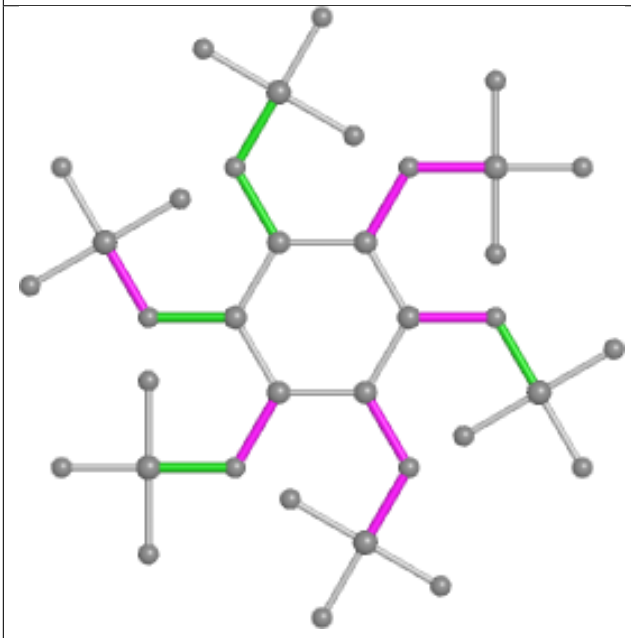
Ligand IHP D 901



Bond lengths



Bond angles



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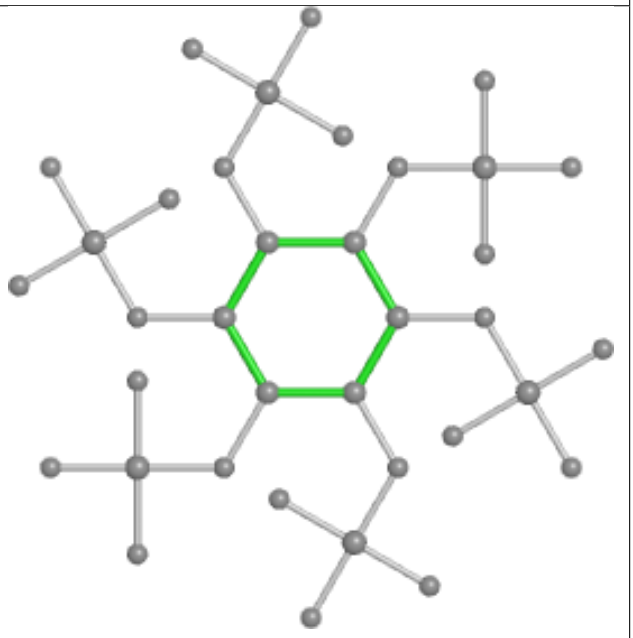
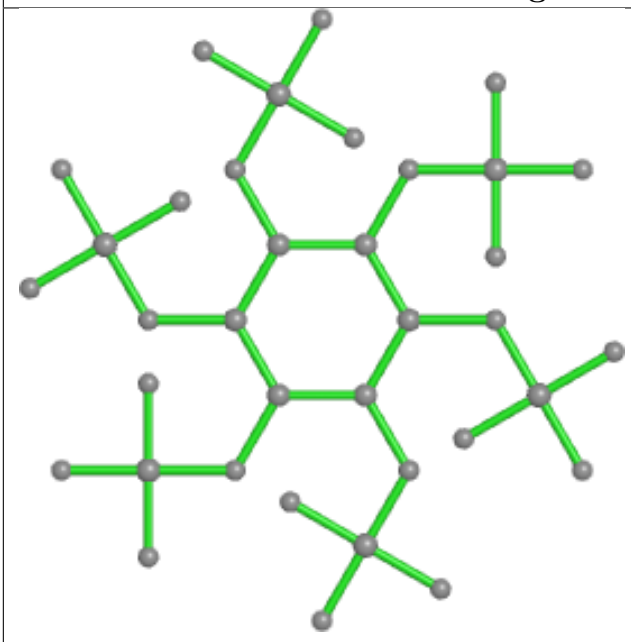


Rings

Ligand IHP B 901



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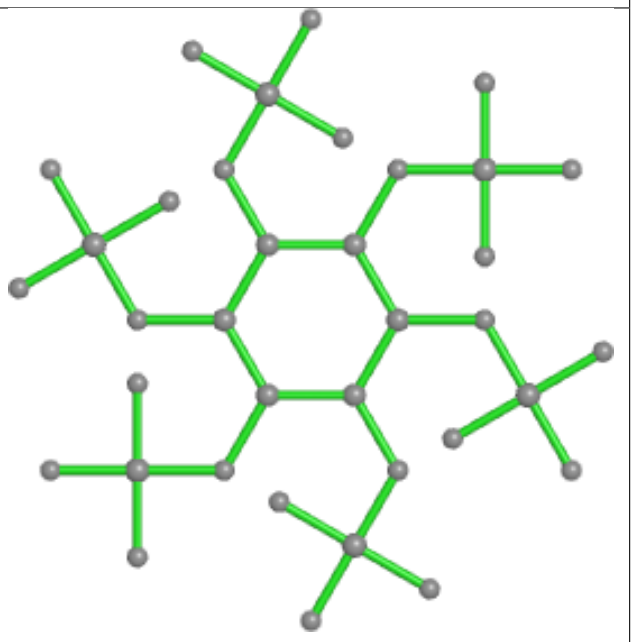
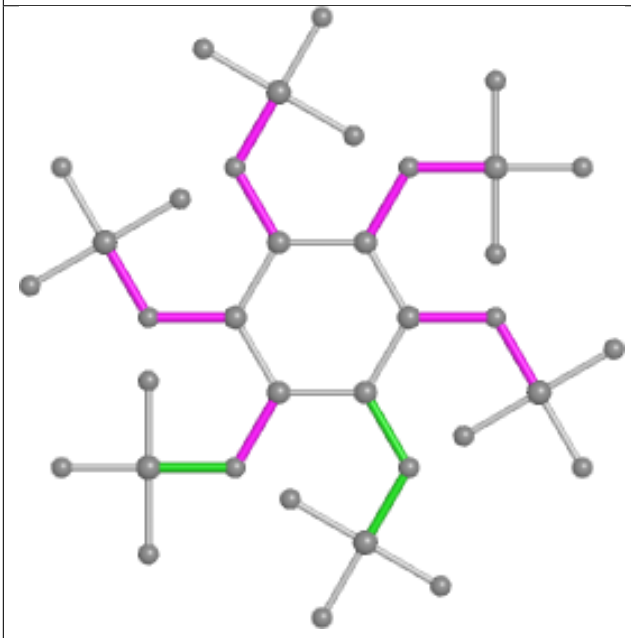


Bond angles



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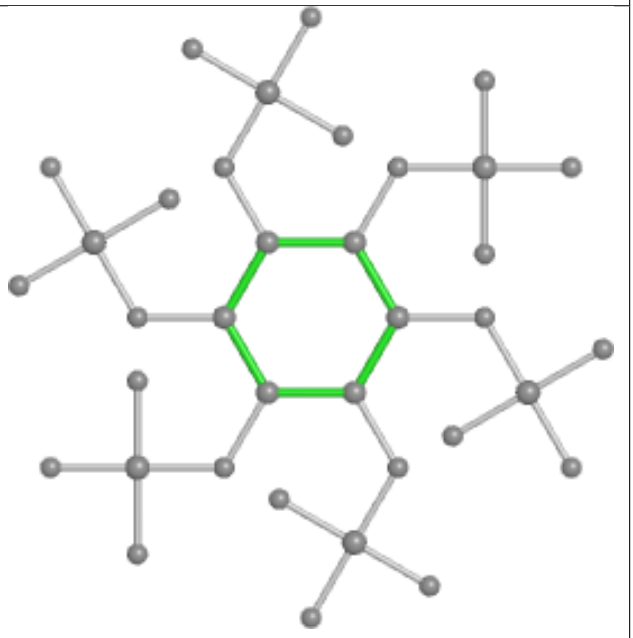
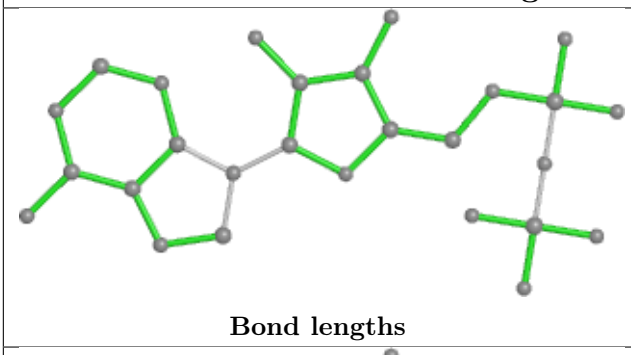
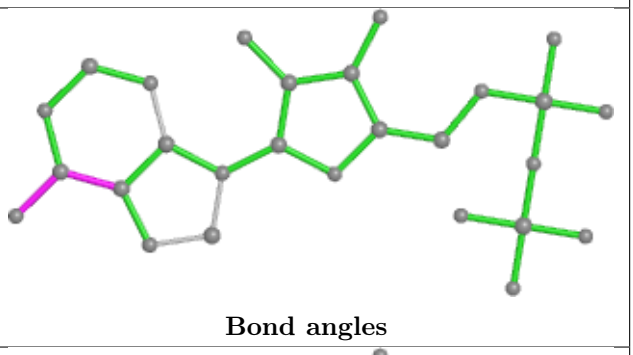


Rings

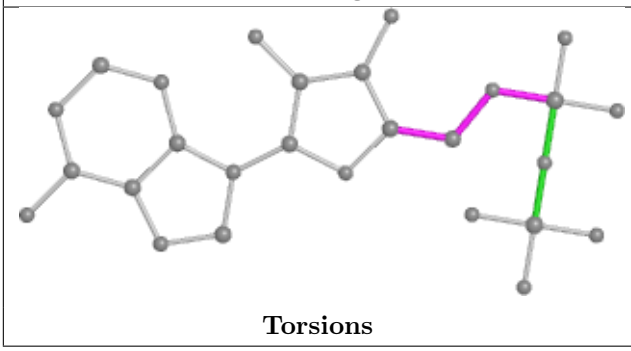
Ligand ADP D 902



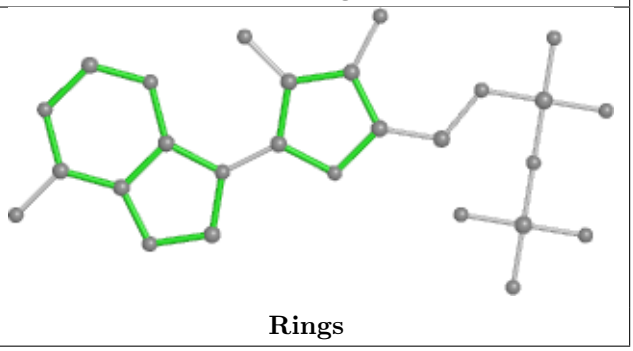
Bond lengths



Bond angles

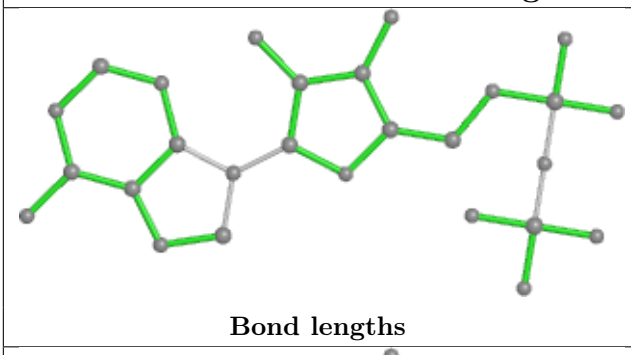


Torsions

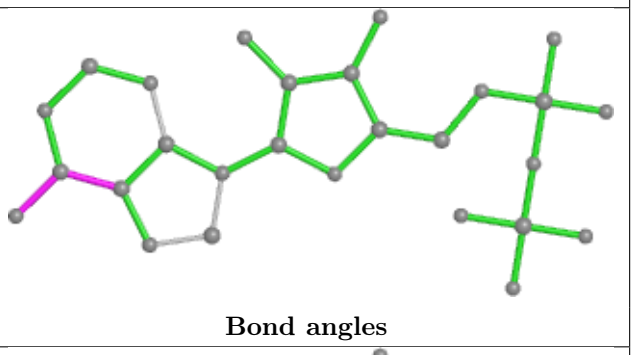


Rings

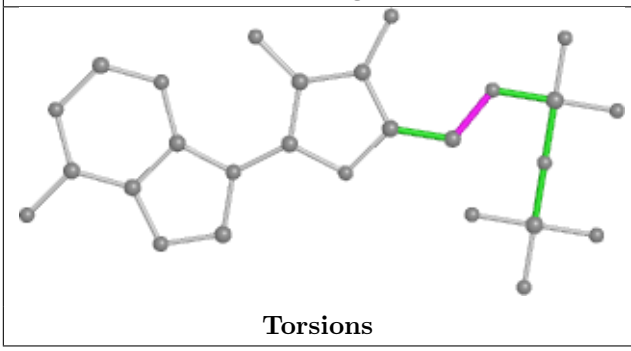
Ligand ADP B 902



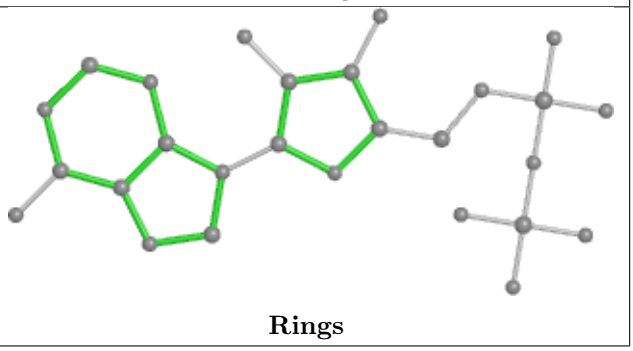
Bond lengths



Bond angles

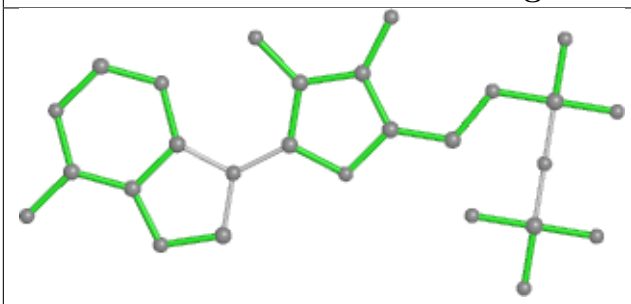


Torsions

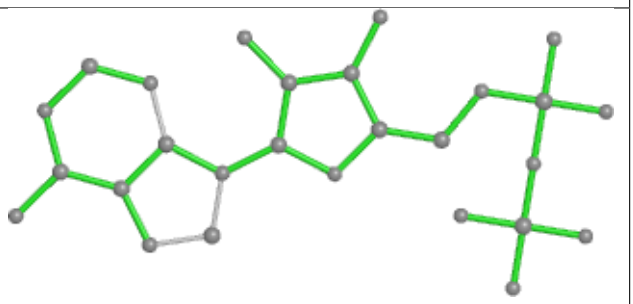


Rings

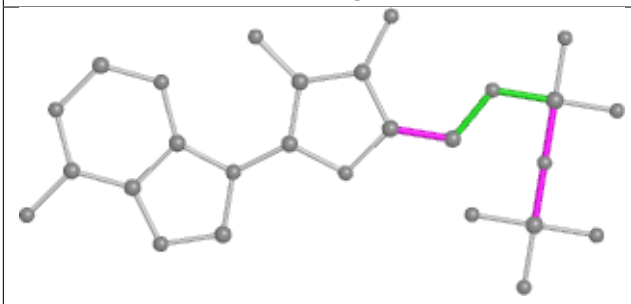
Ligand ADP L 902



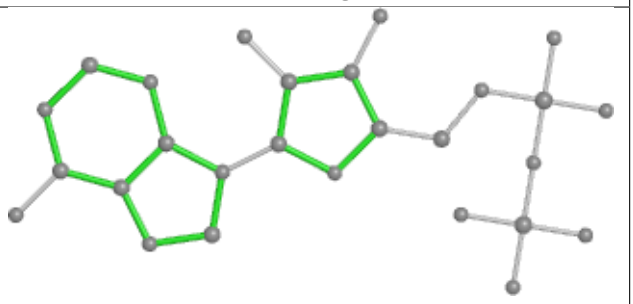
Bond lengths



Bond angles

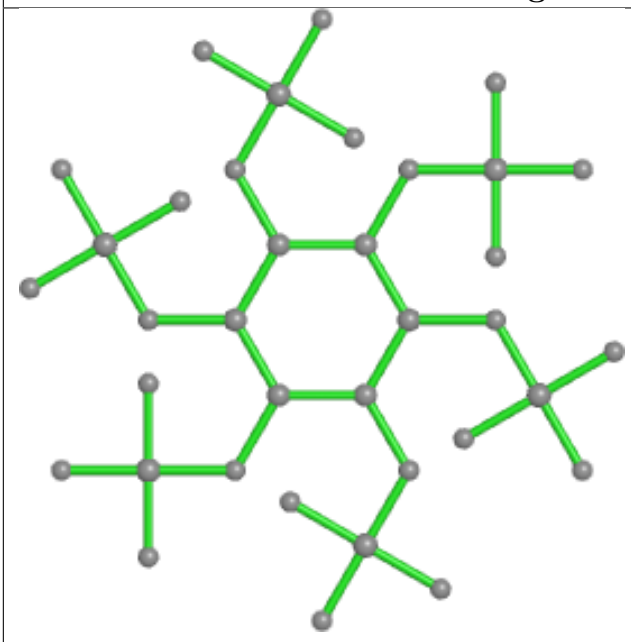


Torsions

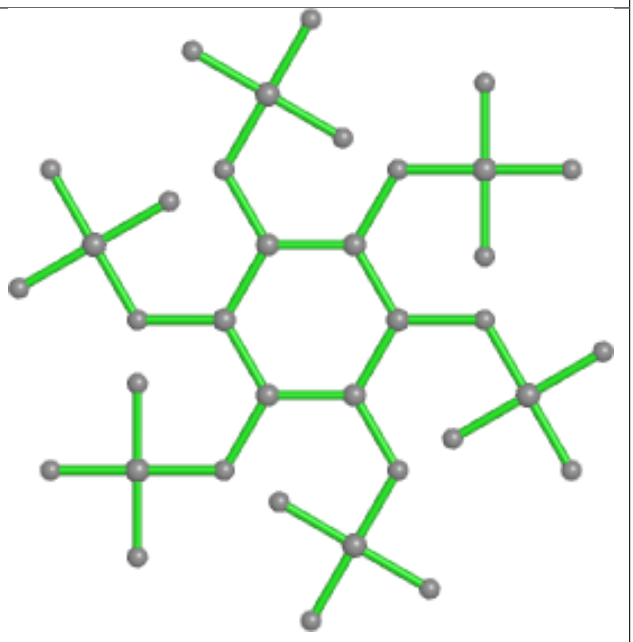


Rings

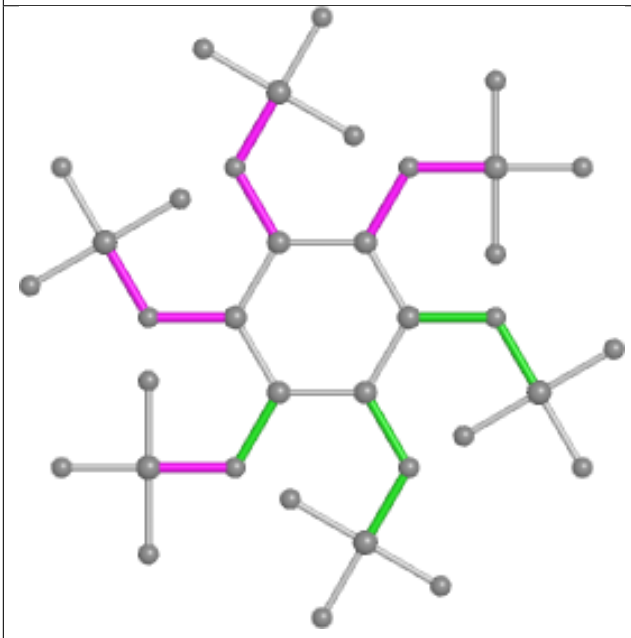
Ligand IHP A 901



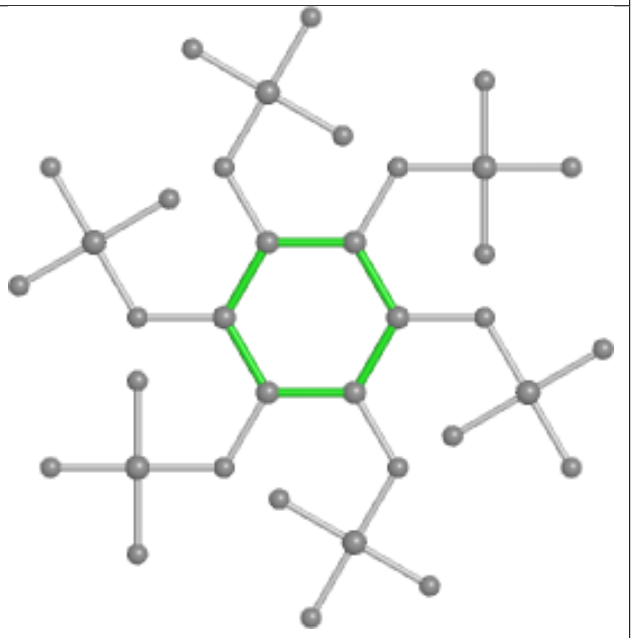
Bond lengths



Bond angles

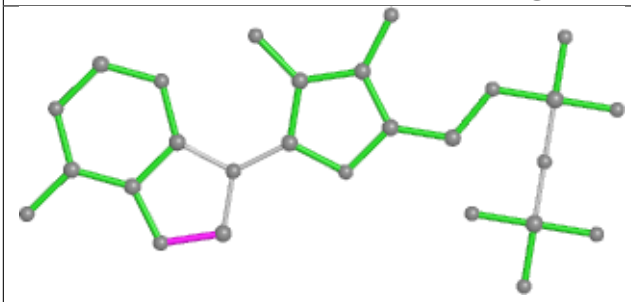


Torsions

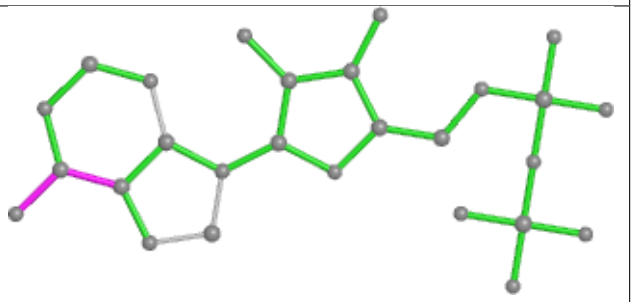


Rings

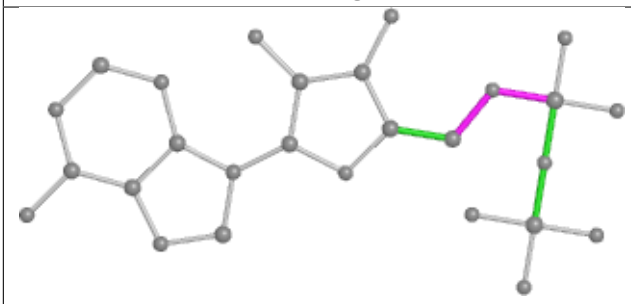
Ligand ADP I 902



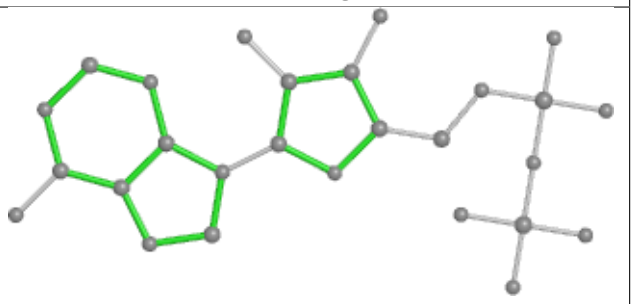
Bond lengths



Bond angles

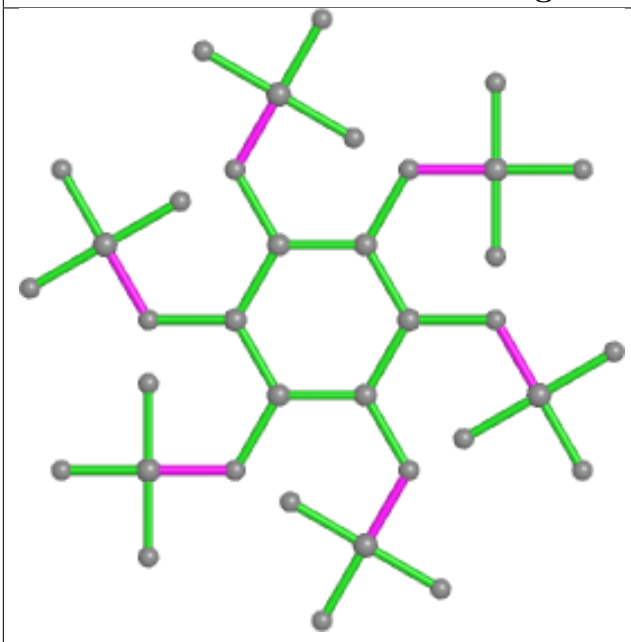


Torsions

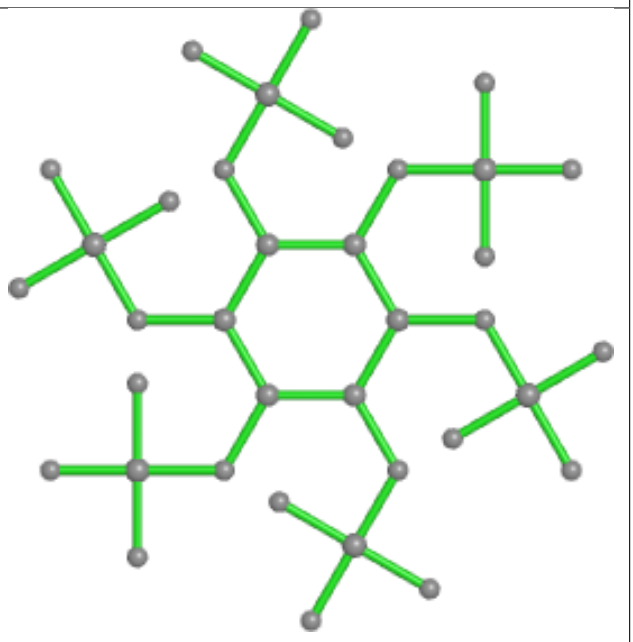


Rings

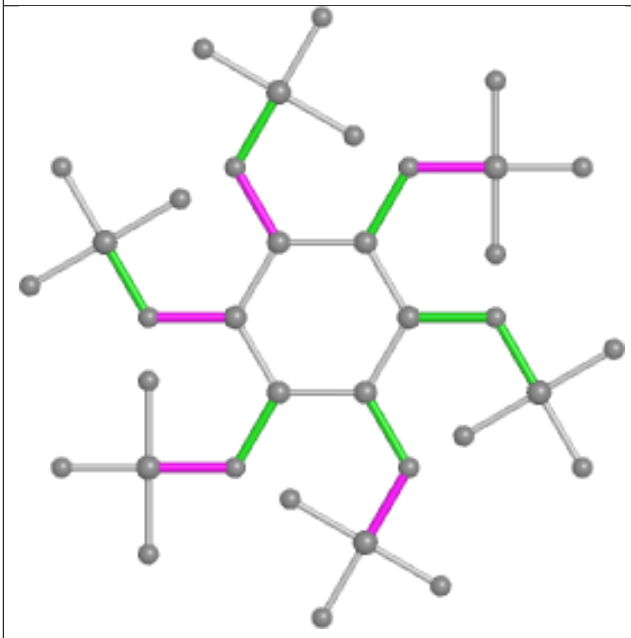
Ligand IHP I 901



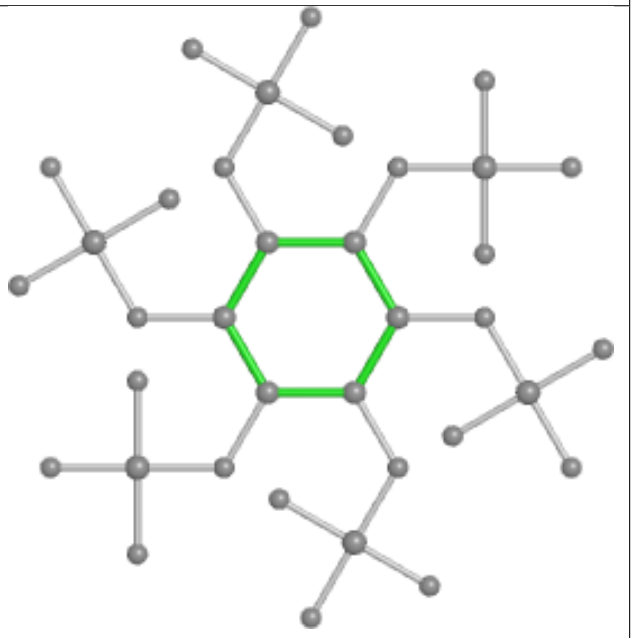
Bond lengths



Bond angles

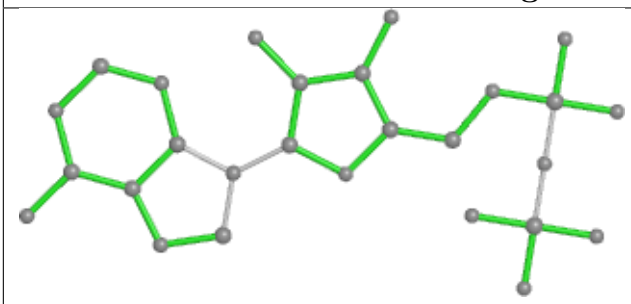


Torsions

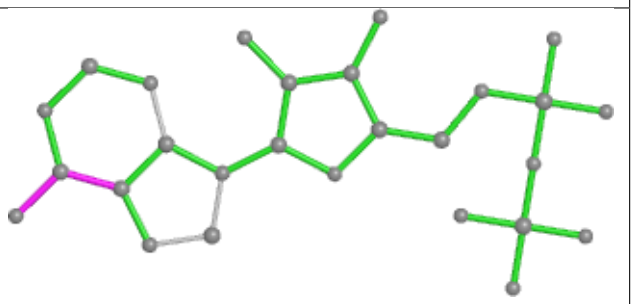


Rings

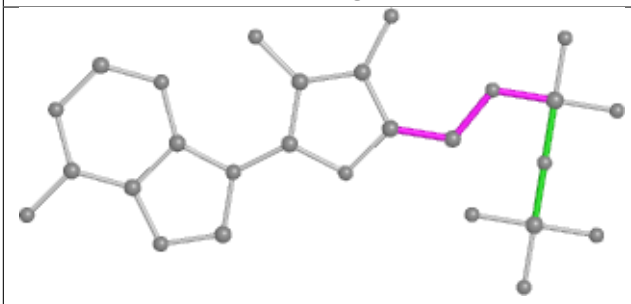
Ligand ADP H 902



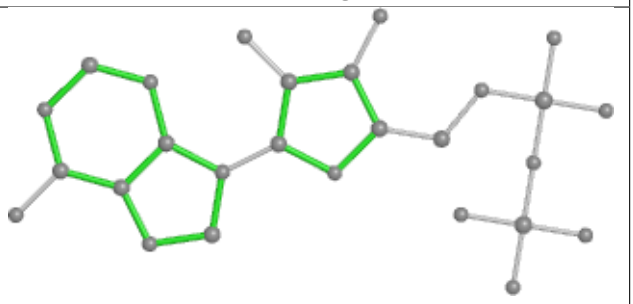
Bond lengths



Bond angles

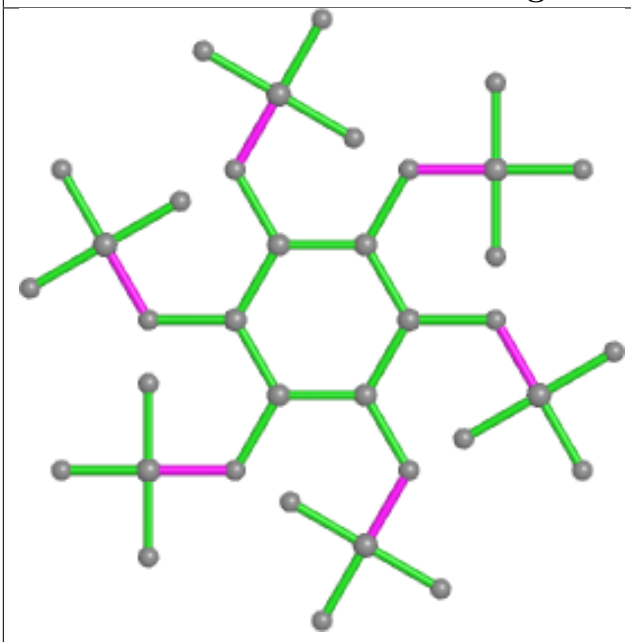


Torsions

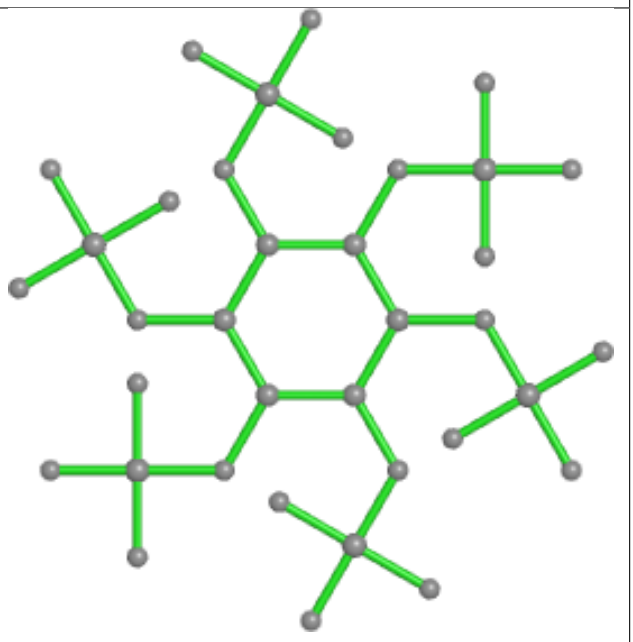


Rings

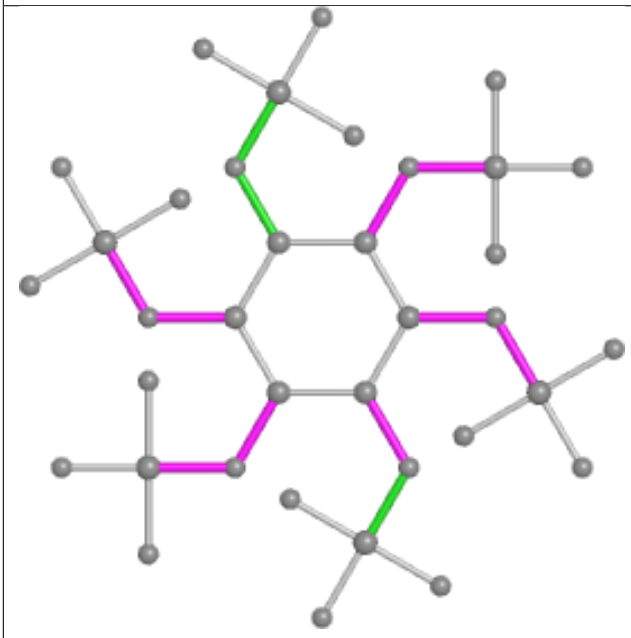
Ligand IHP K 901



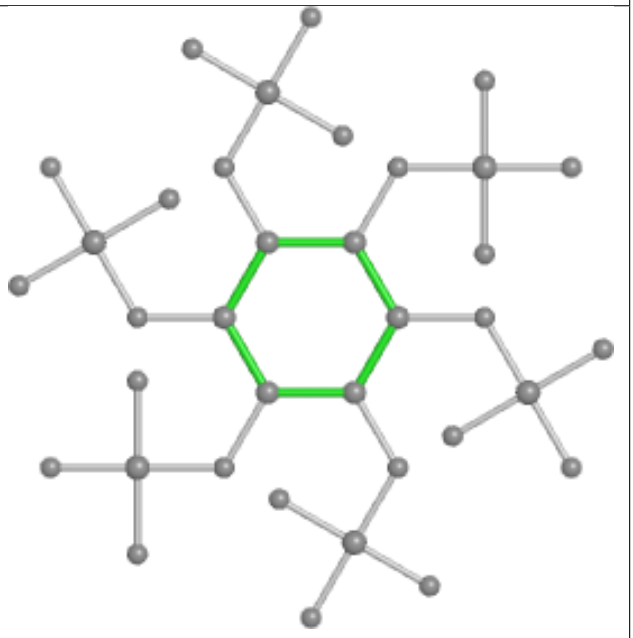
Bond lengths



Bond angles

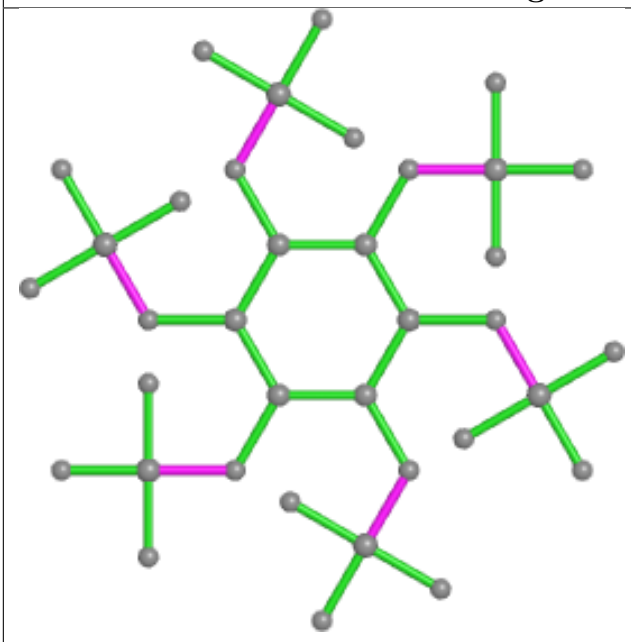


Torsions

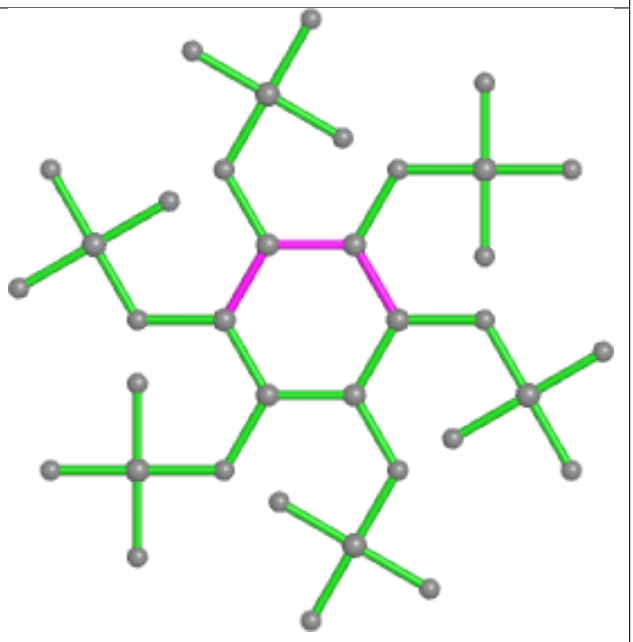


Rings

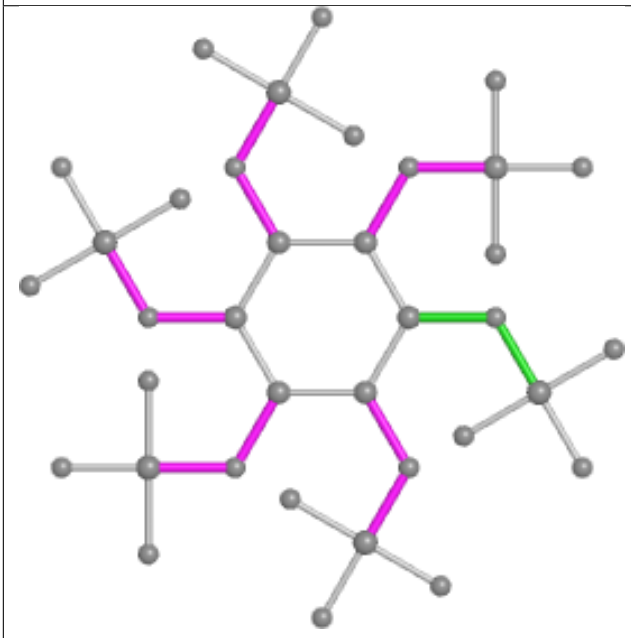
Ligand IHP H 901



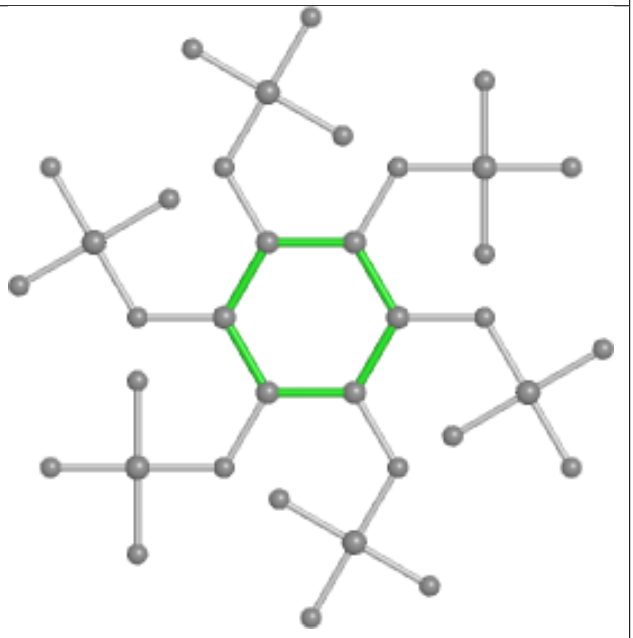
Bond lengths



Bond angles

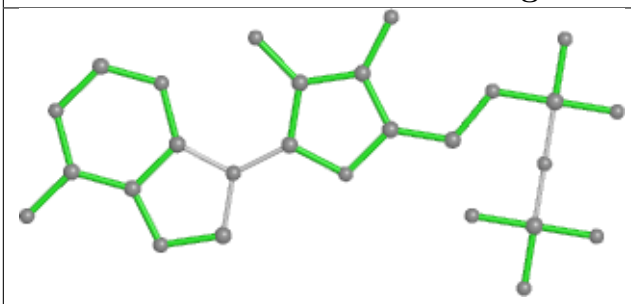


Torsions

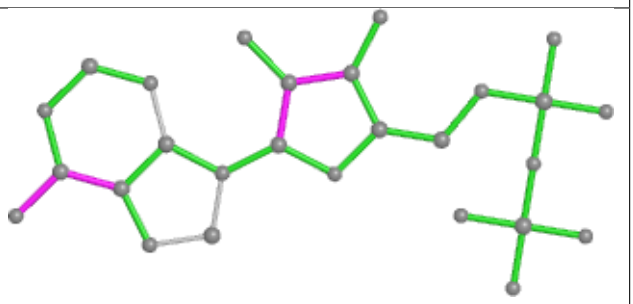


Rings

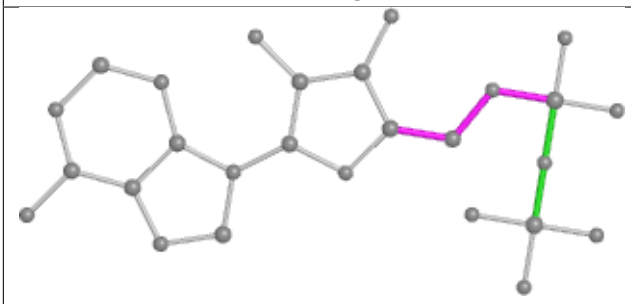
Ligand ADP K 902



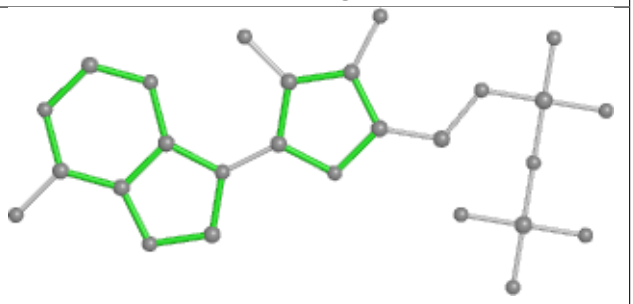
Bond lengths



Bond angles

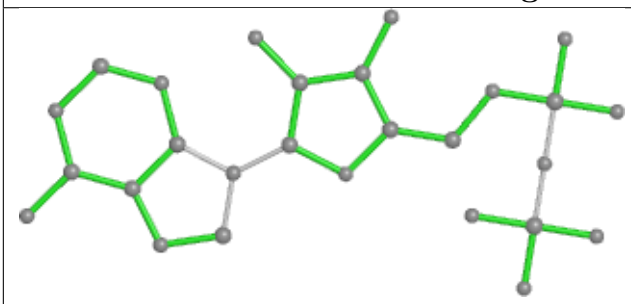


Torsions

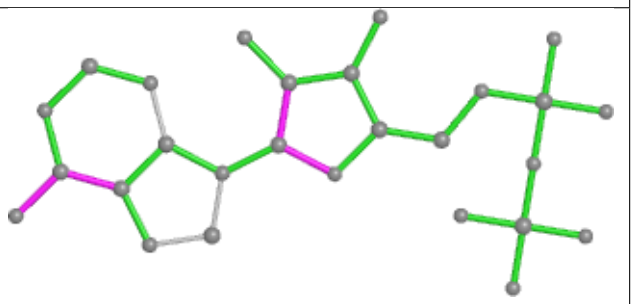


Rings

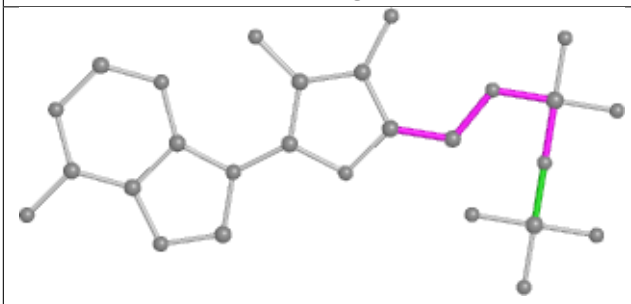
Ligand ADP G 902



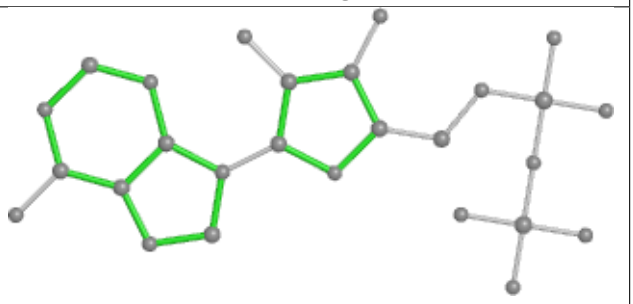
Bond lengths



Bond angles

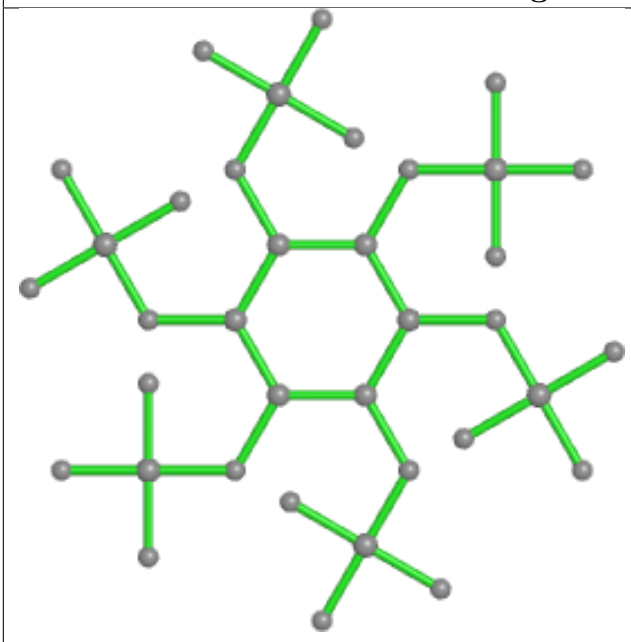


Torsions

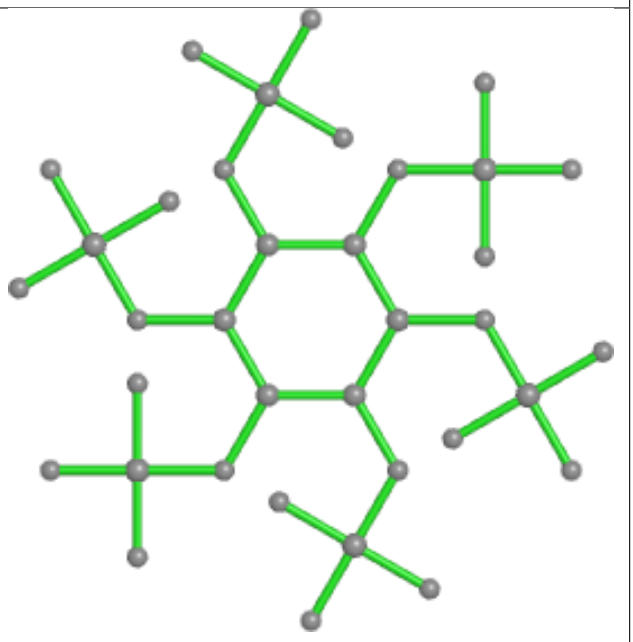


Rings

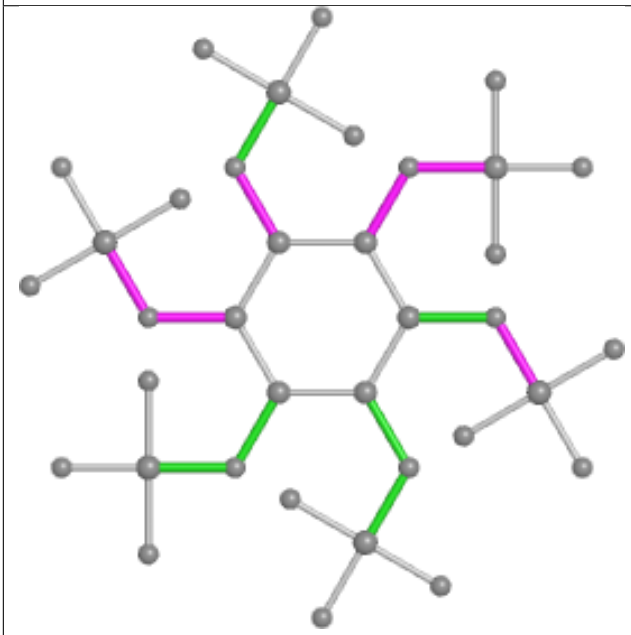
Ligand IHP F 901



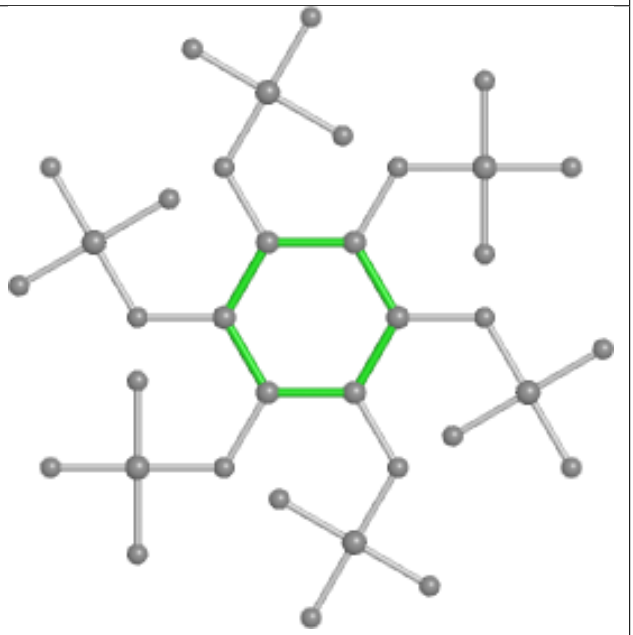
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

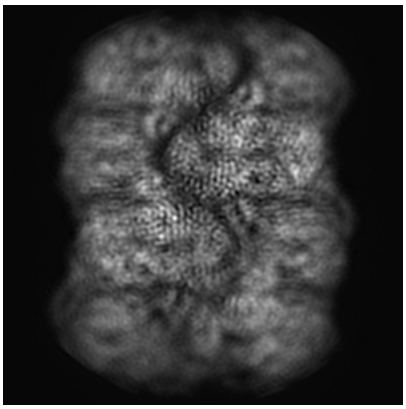
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38685. These allow visual inspection of the internal detail of the map and identification of artifacts.

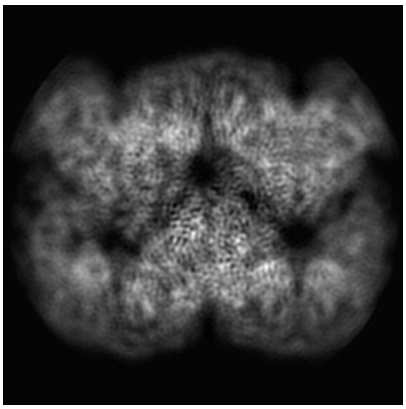
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

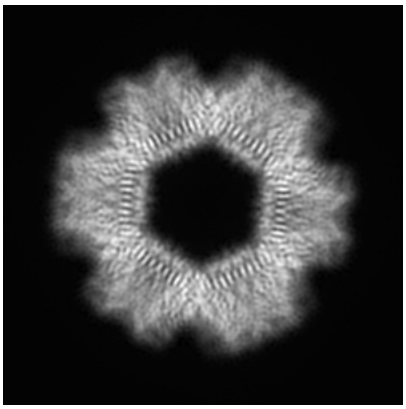
6.1.1 Primary map



X

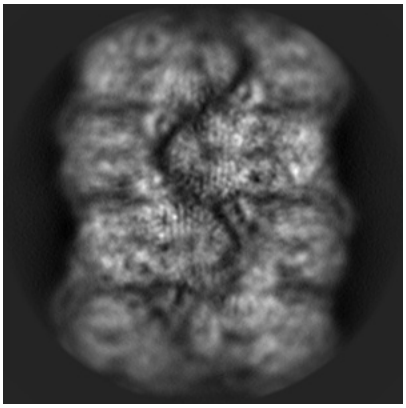


Y

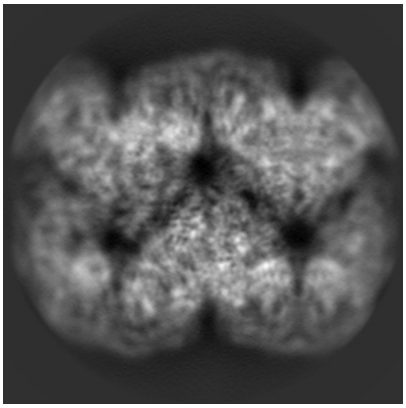


Z

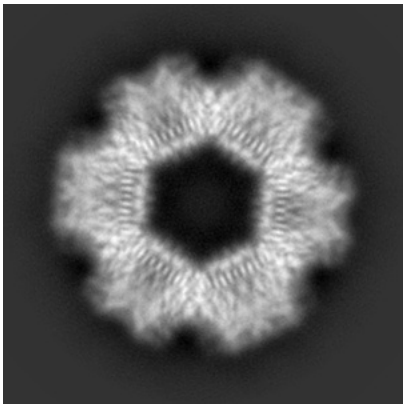
6.1.2 Raw map



X



Y

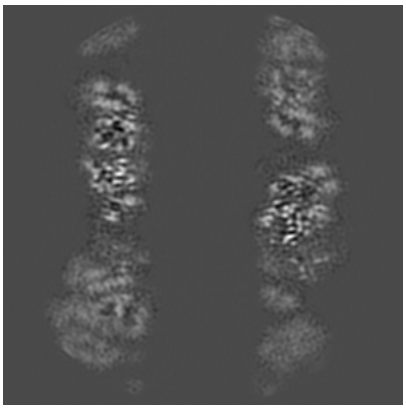


Z

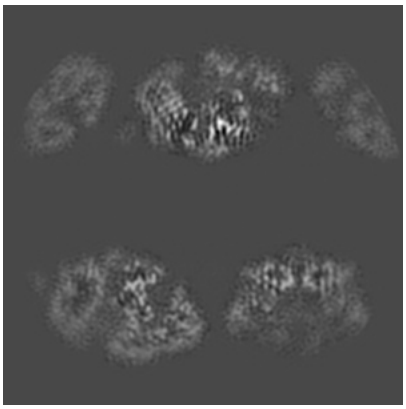
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

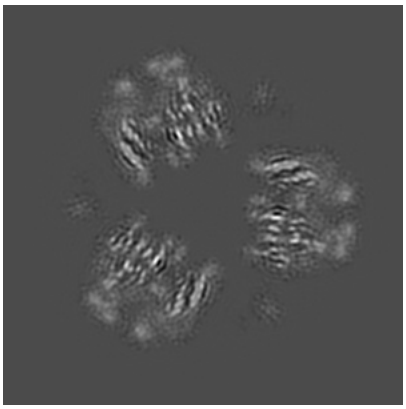
6.2.1 Primary map



X Index: 128

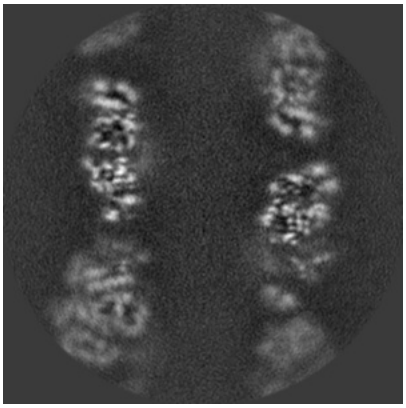


Y Index: 128

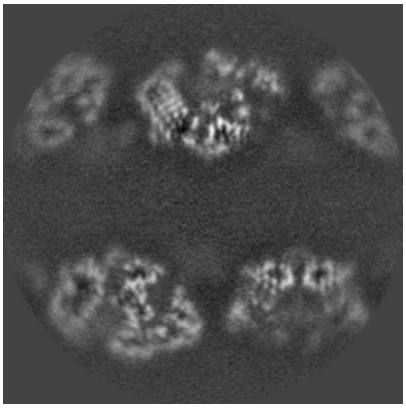


Z Index: 128

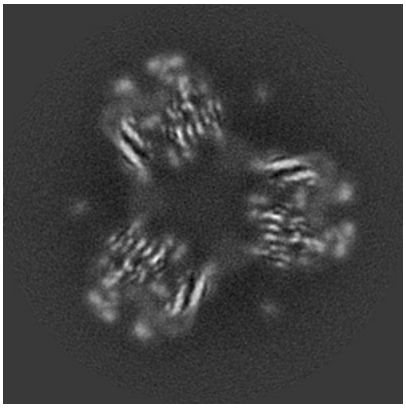
6.2.2 Raw map



X Index: 128



Y Index: 128

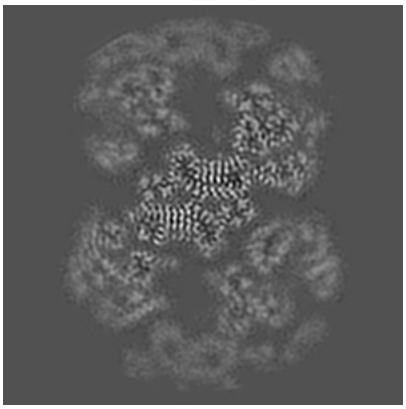


Z Index: 128

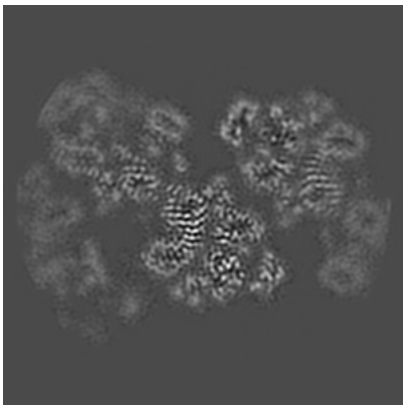
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

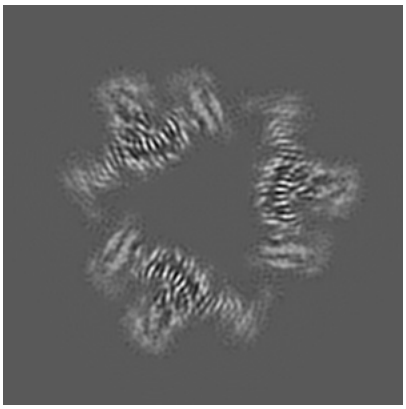
6.3.1 Primary map



X Index: 177

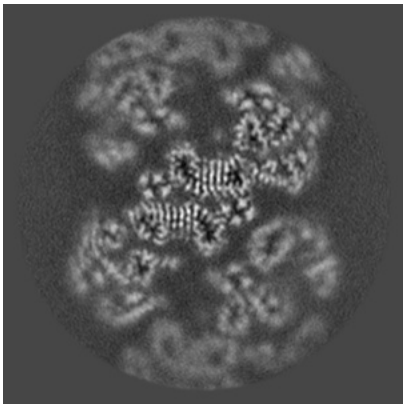


Y Index: 177

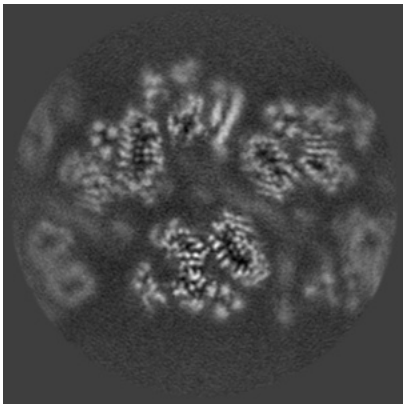


Z Index: 143

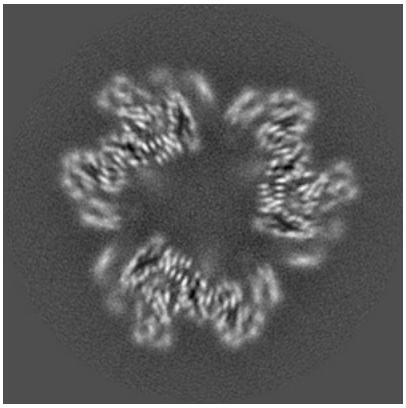
6.3.2 Raw map



X Index: 178



Y Index: 90

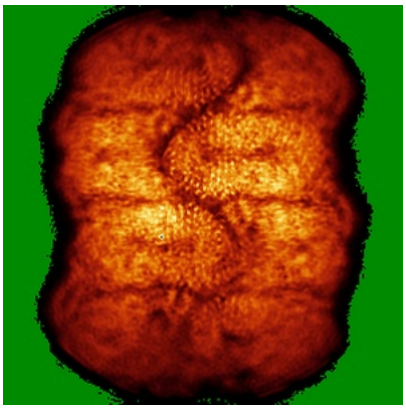


Z Index: 150

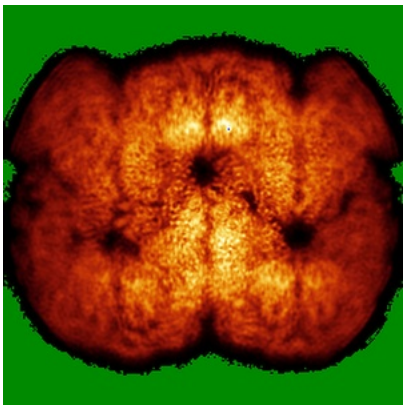
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

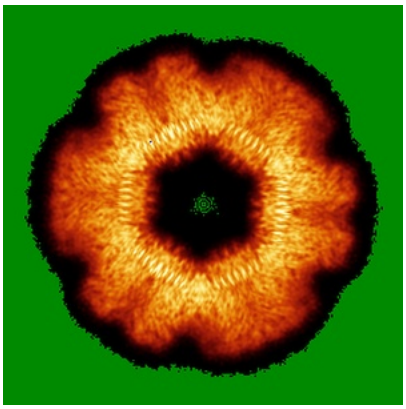
6.4.1 Primary map



X

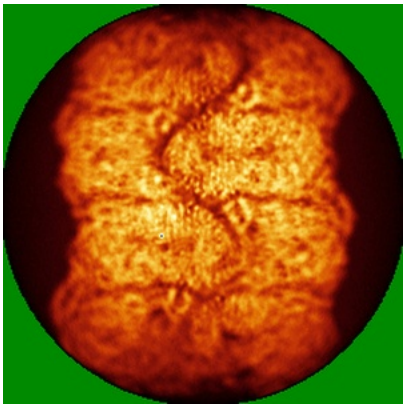


Y

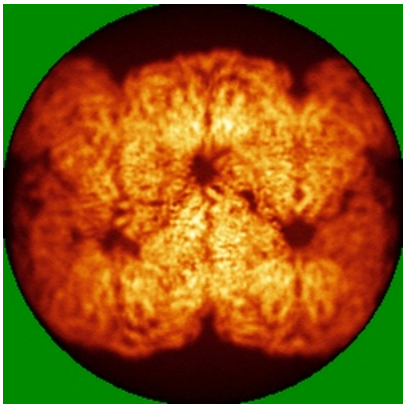


Z

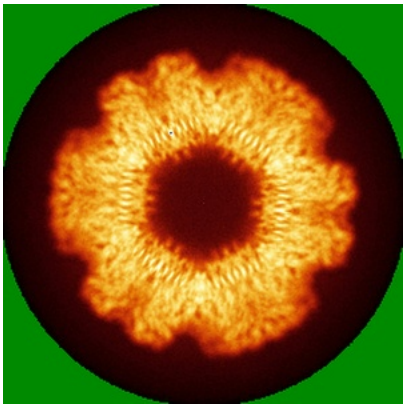
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

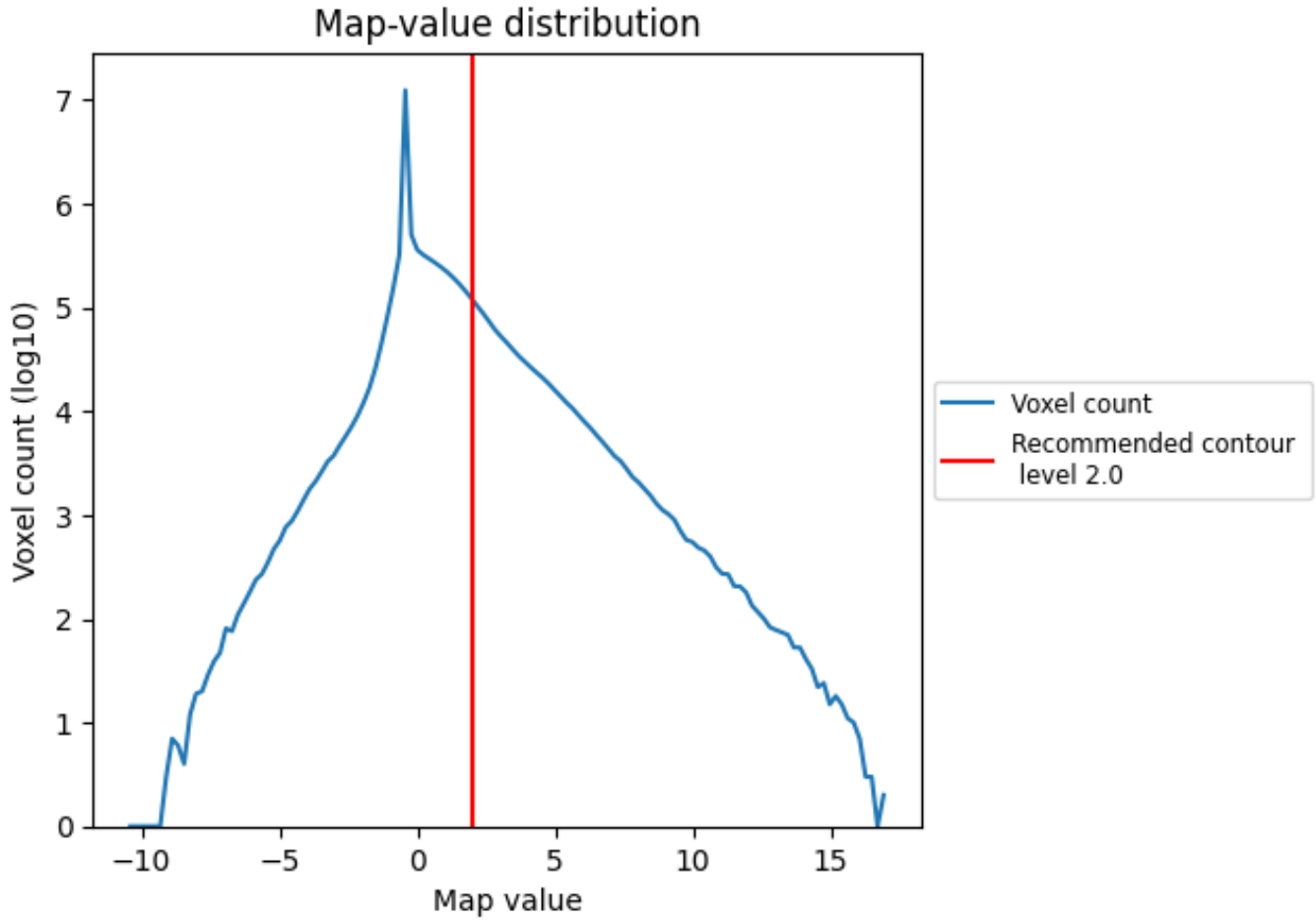
6.6 Mask visualisation (i)

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

7 Map analysis

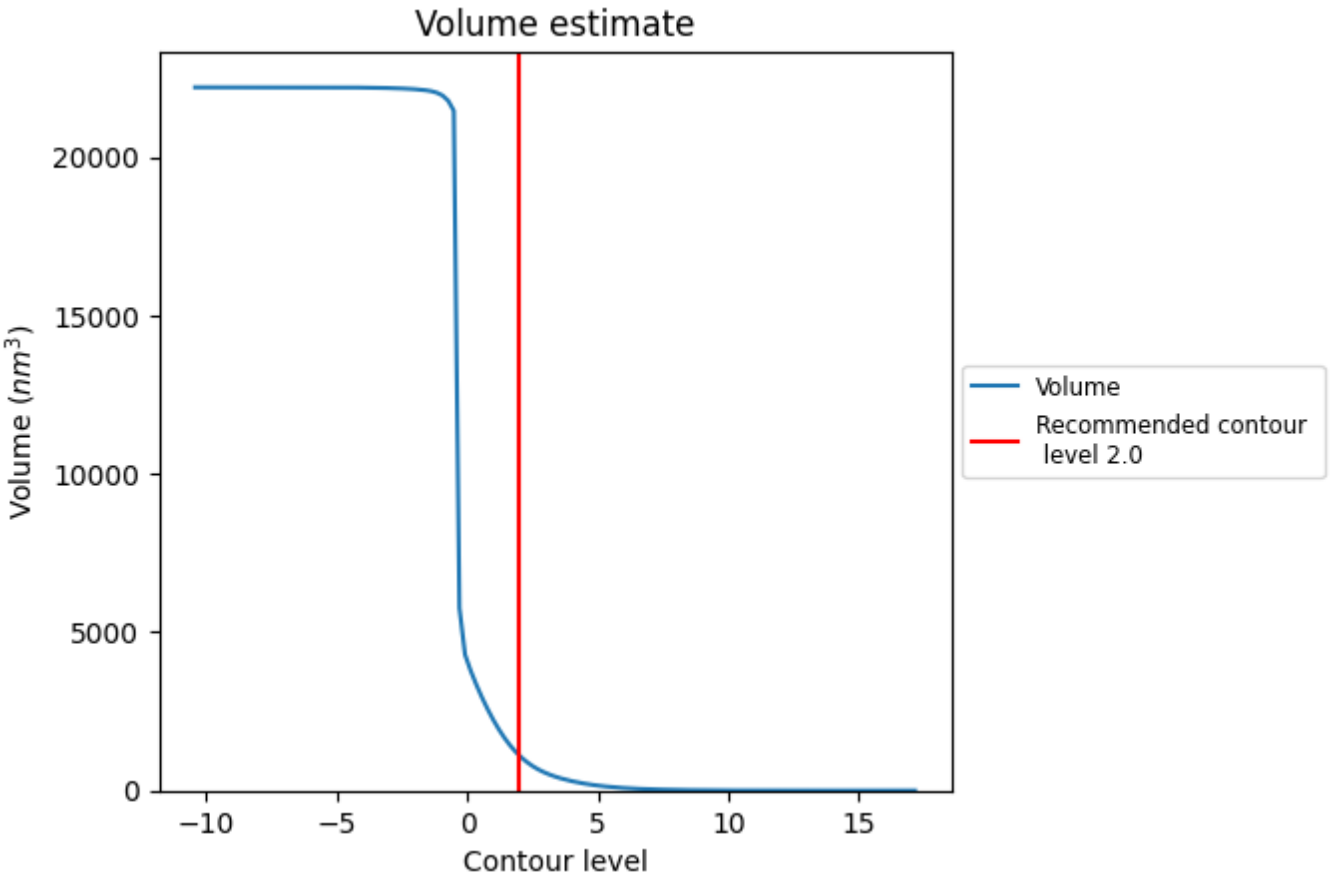
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

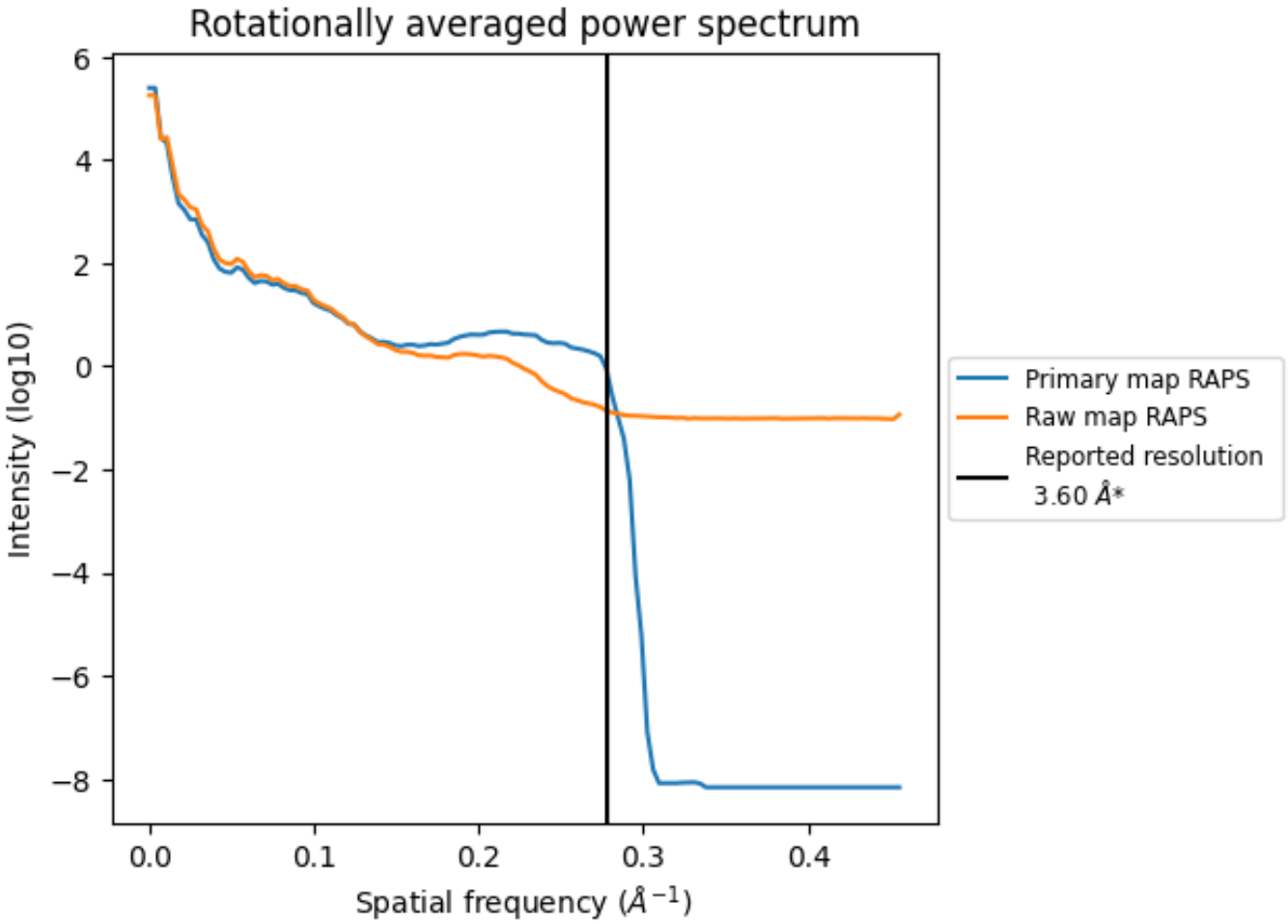
7.2 Volume estimate



The volume at the recommended contour level is 1109 nm^3; this corresponds to an approximate mass of 1002 kDa.

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

7.3 Rotationally averaged power spectrum (i)

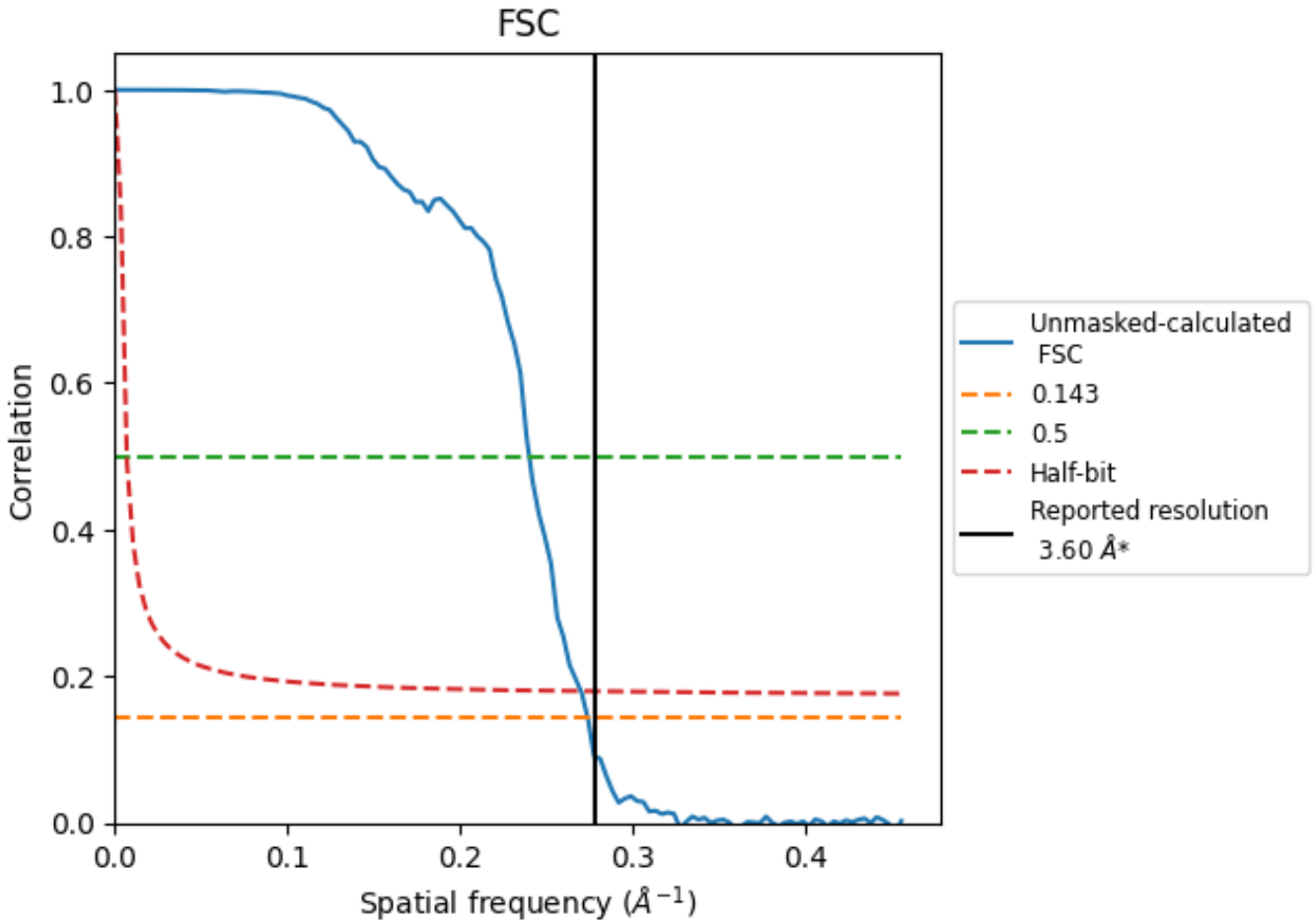


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

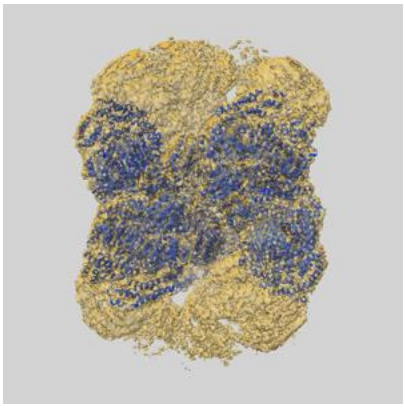
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.17	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

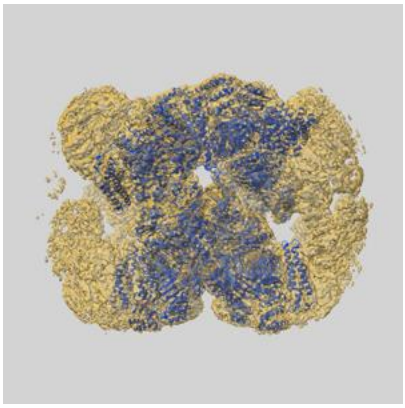
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38685 and PDB model 8XUV. Per-residue inclusion information can be found in section 3 on page 7.

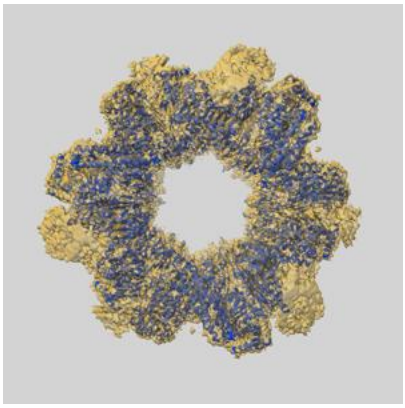
9.1 Map-model overlay



X



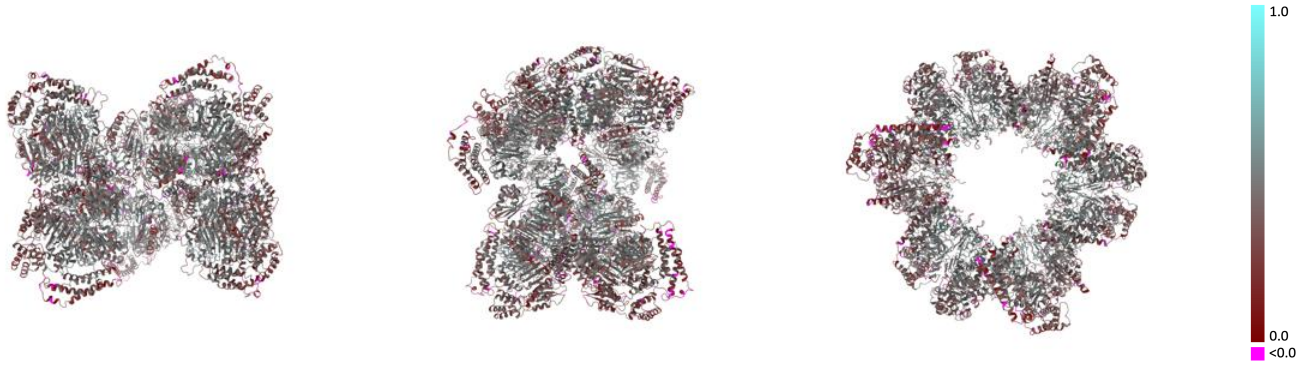
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

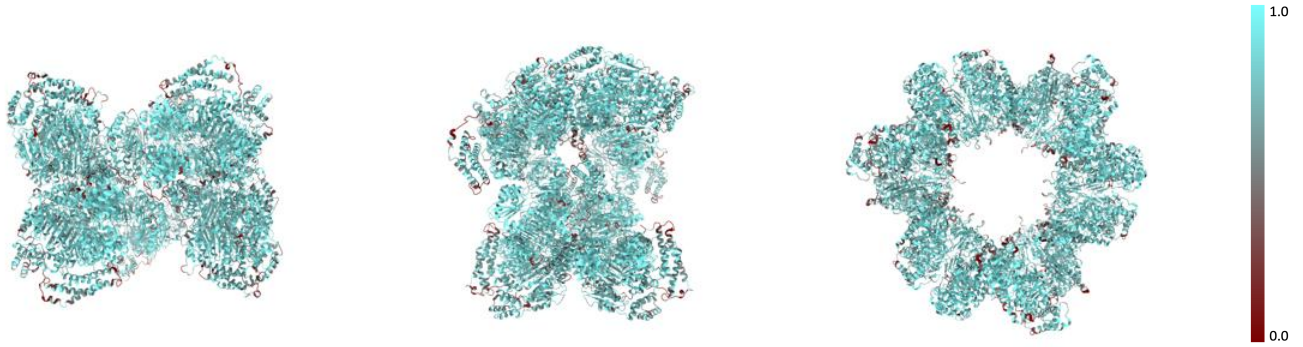
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

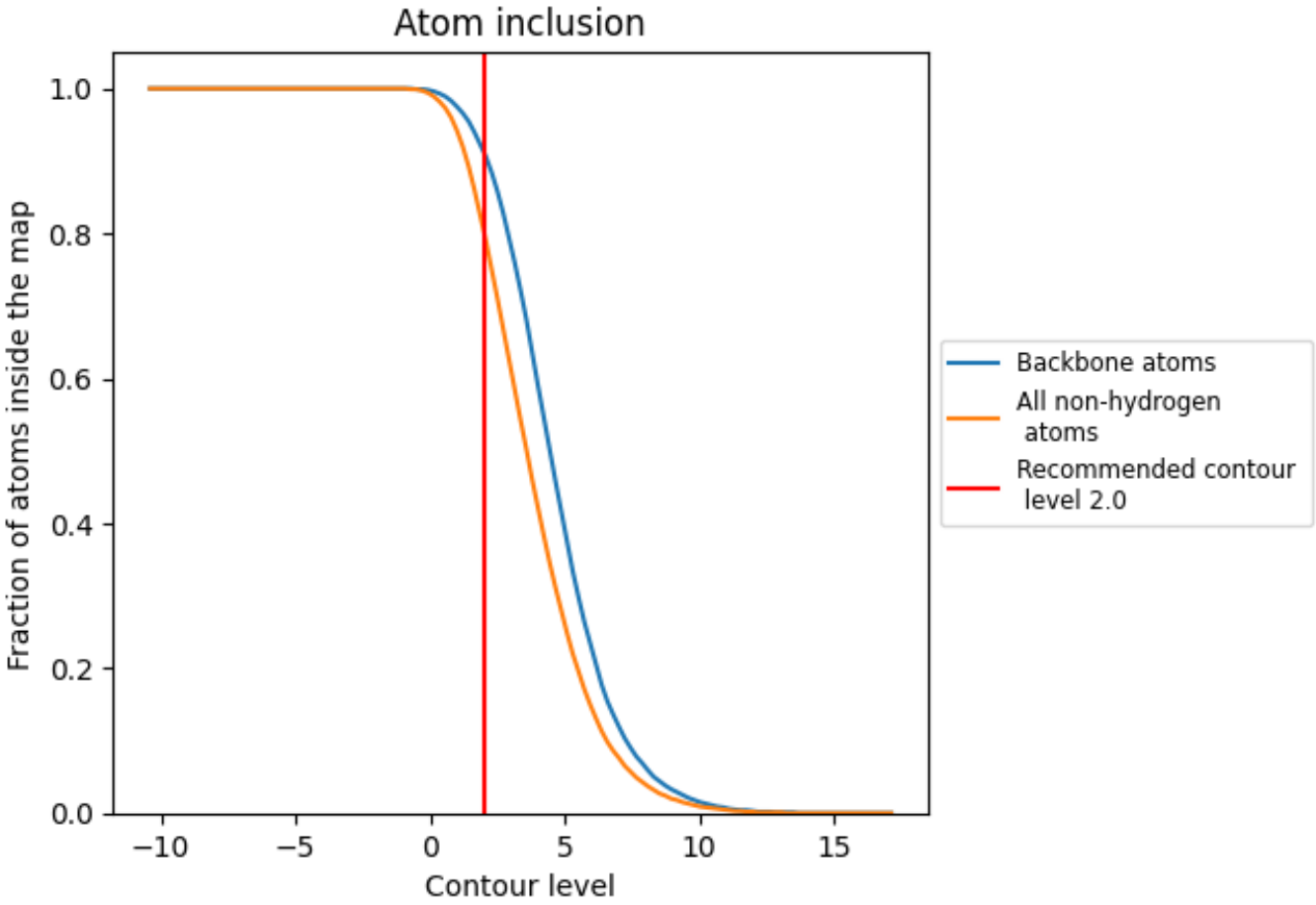
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.4040
A	0.8250	0.4210
B	0.8390	0.4250
C	0.7350	0.3270
D	0.7630	0.3890
E	0.8360	0.4250
F	0.7910	0.4020
G	0.7710	0.3890
H	0.8290	0.4260
I	0.8370	0.4280
J	0.8420	0.4320
K	0.7970	0.4010
L	0.7630	0.3850