Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 01:05 AM EDT

PDB ID	:	1IJJ
Title	:	THE X-RAY CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN RABBIT SKELETAL MUSCLE ACTIN AND LATRUNCULIN A AT 2.85 A RESOLUTION
Authors	:	Vorobiev, S.M.; Bubb, M.R.; Almo, S.C.
Deposited on	:	2001-04-26
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

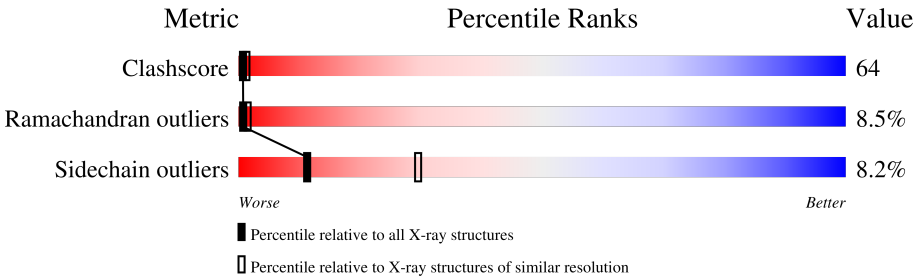
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	27% 58% 10%
1	B	377	31% 56% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5674 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

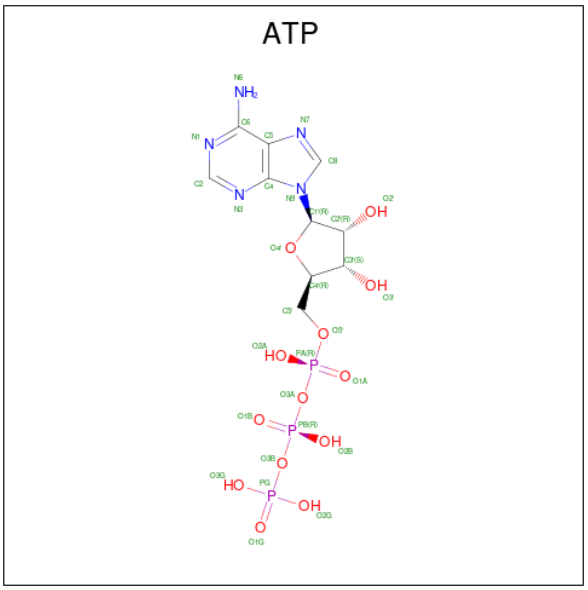
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2714	1722	457	516	19			
1	B	371	Total	C	N	O	S	0	0	0
			2782	1766	468	528	20			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

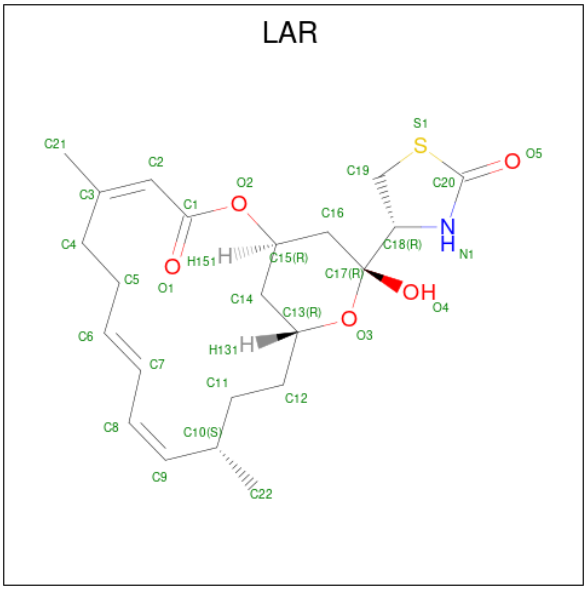
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	15	Total	O	0	0
			15	15		

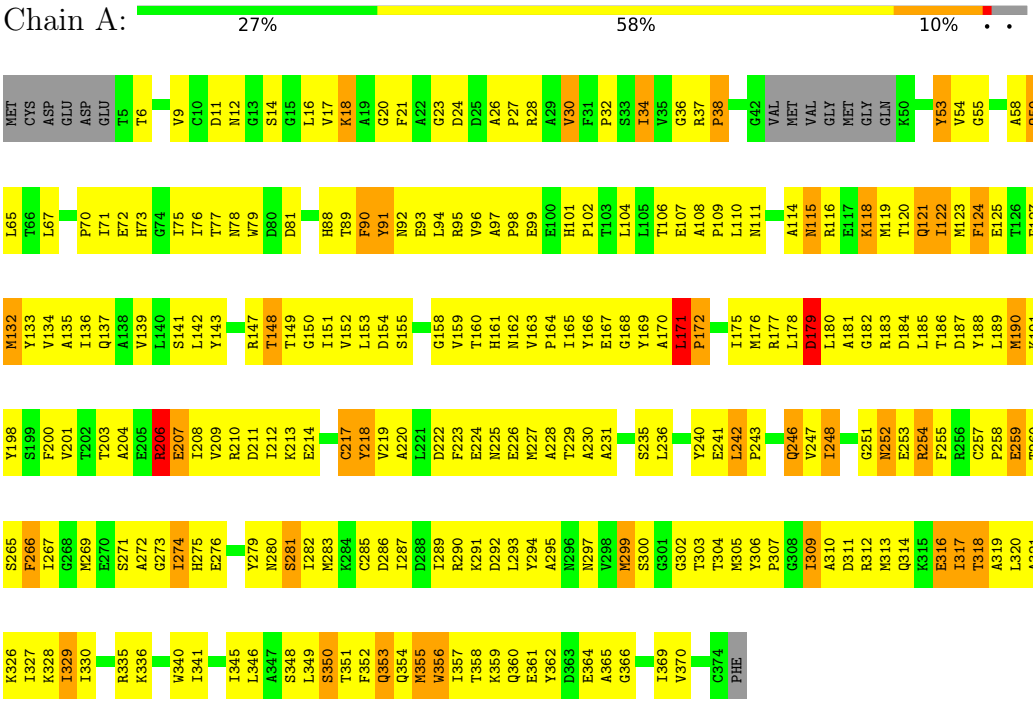
3 Residue-property plots (i)

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

Note EDS was not executed.

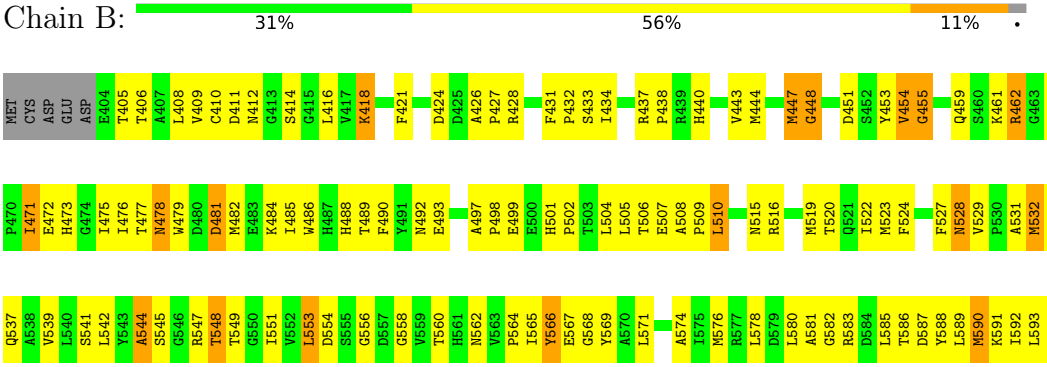
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

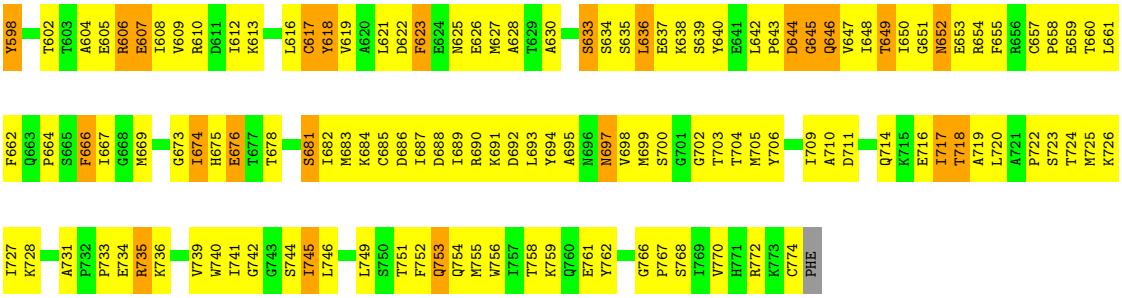
Chain A:



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain B:




Y598 T602 T603 A604 E605 R606 E607 I608 V609 R610 D611 I612 K613 L616 C617 Y618 V619 A620 L621 D622 F623 E624 N625 E626 M627 A628 T629 A630 S633 S634 S635 L636 E637 K638 S639 Y640 E641 L642 P643 D644 G645 Q646 V647 I648 T649 I650 G651 N652 E653 R654 F655 R656 C657 P658 E659 T660 L661
F662 Q663 P664 S665 F666 I667 G668 M669 G673 I674 H675 E676 T677 T678 S681 I682 M683 K684 C685 D686 I687 D688 I689 R690 K691 D692 L693 Y694 A695 N696 N697 V698 M699 S700 G701 G702 T703 T704 M705 Y706 I709 A710 D711 Q714 K715 E716 I717 T718 A719 L720 A721 P722 S723 T724 M725 K726
I727 K728 A731 P732 P733 E734 R735 K736 V739 W740 I741 G742 G743 S744 I745 L746 L749 S750 T751 F752 Q753 Q754 M755 W756 I757 T758 K759 Q760 E761 Y762 G766 P767 S768 I769 V770 H771 R772 K773 C774 PHE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.30Å 102.18Å 124.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.85	Depositor
% Data completeness (in resolution range)	96.9 (15.00-2.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5674	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.80	1/2773 (0.0%)	0.98	2/3777 (0.1%)
1	B	0.79	1/2844 (0.0%)	0.97	5/3874 (0.1%)
All	All	0.80	2/5617 (0.0%)	0.97	7/7651 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	774	CYS	C-O	-8.26	1.07	1.23
1	A	356	TRP	CB-CG	-5.04	1.41	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	LEU	CA-CB-CG	-9.46	93.55	115.30
1	B	774	CYS	CA-C-O	8.81	138.59	120.10
1	B	571	LEU	CA-CB-CG	-7.82	97.32	115.30
1	A	200	PHE	N-CA-C	-5.63	95.80	111.00
1	B	510	LEU	CA-CB-CG	-5.32	103.08	115.30
1	B	726	LYS	N-CA-C	-5.02	97.44	111.00
1	B	649	THR	N-CA-CB	5.02	119.83	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2714	0	2584	344	0
1	B	2782	0	2652	353	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	4	0
4	A	29	0	31	6	0
4	B	29	0	31	10	0
5	A	41	0	0	1	0
5	B	15	0	0	0	0
All	All	5674	0	5322	695	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 64.

All (695) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HB3	1:A:209:VAL:HG11	1.26	1.16
1:B:590:MET:CG	1:B:609:VAL:HG11	1.79	1.13
1:B:588:TYR:HE2	1:B:657:CYS:HA	1.03	1.09
1:B:588:TYR:CE2	1:B:657:CYS:HA	1.88	1.08
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.30	1.07
1:B:596:ARG:HB3	1:B:598:TYR:HE1	1.14	1.06
1:A:59:GLN:HE21	1:A:59:GLN:HA	1.18	1.04
1:B:582:GLY:HA2	1:B:703:THR:HG21	1.35	1.04
1:B:472:GLU:HG3	1:B:477:THR:HG21	1.41	1.03
1:B:590:MET:HG2	1:B:609:VAL:HG11	1.40	1.03
1:B:609:VAL:HA	1:B:612:ILE:HD12	1.40	1.02
1:B:532:MET:HG2	1:B:533:TYR:N	1.72	1.00
1:A:329:ILE:H	1:A:329:ILE:HD13	1.22	0.99
1:B:596:ARG:HH12	1:B:651:GLY:HA3	1.26	0.98
1:A:329:ILE:HD13	1:A:329:ILE:N	1.78	0.98
1:B:593:LEU:HD23	1:B:609:VAL:HG23	1.41	0.98
1:A:366:GLY:O	1:A:369:ILE:HG22	1.60	0.98
1:B:412:ASN:HD21	1:B:486:TRP:HE1	1.09	0.97
1:A:230:ALA:HB2	1:A:236:LEU:HD13	1.49	0.94
1:B:589:LEU:HG	1:B:593:LEU:HD22	1.48	0.94
1:B:589:LEU:O	1:B:593:LEU:HB2	1.66	0.94
1:A:241:GLU:HA	1:A:246:GLN:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:VAL:HA	1:B:612:ILE:CD1	1.98	0.93
1:A:228:ALA:HA	1:A:231:ALA:HB3	1.51	0.93
1:B:472:GLU:HG3	1:B:477:THR:CG2	1.99	0.92
1:A:273:GLY:O	1:A:276:GLU:HB2	1.71	0.91
1:B:717:ILE:HG22	1:B:727:ILE:HD13	1.52	0.90
1:B:481:ASP:O	1:B:484:LYS:HB2	1.72	0.90
1:B:589:LEU:HD12	1:B:592:ILE:HD11	1.53	0.90
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.50	0.90
1:B:412:ASN:ND2	1:B:486:TRP:HE1	1.70	0.88
1:B:596:ARG:HB3	1:B:598:TYR:CE1	2.07	0.87
1:A:59:GLN:HA	1:A:59:GLN:NE2	1.90	0.87
1:B:590:MET:HG3	1:B:609:VAL:HG11	1.55	0.86
1:B:661:LEU:HB3	1:B:674:ILE:HD11	1.55	0.86
1:A:219:VAL:HG11	1:A:309:ILE:HA	1.58	0.85
1:B:704:THR:O	1:B:735:ARG:NH1	2.09	0.85
1:B:565:ILE:HA	1:B:569:TYR:O	1.76	0.85
1:A:212:ILE:HG12	1:A:240:TYR:CE2	2.12	0.85
1:B:602:THR:HG23	1:B:605:GLU:H	1.40	0.85
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.59	0.85
1:B:639:SER:HB3	1:B:649:THR:HG22	1.58	0.84
1:B:618:TYR:O	1:B:655:PHE:HA	1.77	0.84
1:A:38:PRO:HA	1:A:65:LEU:HD23	1.59	0.84
1:A:148:THR:O	1:A:168:GLY:N	2.11	0.84
1:B:618:TYR:O	1:B:658:PRO:HG2	1.77	0.84
1:B:616:LEU:HD13	1:B:650:ILE:HG13	1.58	0.83
1:B:642:LEU:HG	1:B:646:GLN:O	1.78	0.83
1:B:582:GLY:CA	1:B:703:THR:HG21	2.09	0.82
1:B:593:LEU:CD2	1:B:609:VAL:HG23	2.10	0.82
1:A:149:THR:OG1	1:A:167:GLU:N	2.13	0.82
1:B:699:MET:CE	1:B:731:ALA:HB2	2.10	0.82
1:B:520:THR:HA	1:B:532:MET:HE3	1.60	0.81
1:A:358:THR:OG1	1:A:361:GLU:HG3	1.80	0.81
1:A:53:TYR:O	1:A:58:ALA:HB2	1.81	0.81
1:B:414:SER:HA	1:B:471:ILE:HG22	1.63	0.81
1:B:718:THR:HA	1:B:727:ILE:HD12	1.63	0.80
1:A:198:TYR:OH	1:A:248:ILE:HG13	1.81	0.80
1:B:598:TYR:N	1:B:598:TYR:CD1	2.48	0.80
1:B:673:GLY:O	1:B:676:GLU:HB2	1.82	0.79
1:B:674:ILE:HG22	1:B:675:HIS:N	1.96	0.79
1:A:132:MET:HG2	1:A:133:TYR:N	1.96	0.79
1:B:613:LYS:HA	1:B:617:CYS:SG	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ILE:HA	1:B:595:GLU:HG2	1.63	0.79
1:B:562:ASN:HB2	1:B:576:MET:HB2	1.65	0.78
1:A:302:GLY:O	1:A:305:MET:HB2	1.84	0.78
1:B:549:THR:HA	1:B:565:ILE:O	1.82	0.78
1:A:110:LEU:HD21	1:A:175:ILE:HD12	1.64	0.78
1:B:604:ALA:O	1:B:608:ILE:HG12	1.82	0.78
1:A:252:ASN:C	1:A:252:ASN:HD22	1.87	0.78
1:B:642:LEU:HD21	1:B:648:ILE:HD11	1.66	0.77
1:B:416:LEU:HB2	1:B:418:LYS:HE2	1.65	0.77
1:A:213:LYS:HA	1:A:217:CYS:SG	2.25	0.77
1:A:208:ILE:O	1:A:212:ILE:HG13	1.84	0.77
1:A:190:MET:HB3	1:A:209:VAL:CG1	2.10	0.77
1:B:414:SER:HA	1:B:471:ILE:CG2	2.15	0.77
1:B:585:LEU:HD11	1:B:661:LEU:HG	1.67	0.76
1:B:638:LYS:HG3	1:B:639:SER:H	1.49	0.76
1:B:678:THR:O	1:B:682:ILE:HD12	1.86	0.76
1:A:165:ILE:HG23	1:A:170:ALA:N	2.00	0.75
1:B:683:MET:O	1:B:685:CYS:N	2.19	0.75
1:A:36:GLY:CA	1:A:67:LEU:HD23	2.16	0.75
1:A:115:ASN:O	1:A:119:MET:HG3	1.86	0.75
1:B:617:CYS:HA	1:B:654:ARG:HG2	1.66	0.75
1:B:661:LEU:HB3	1:B:674:ILE:CD1	2.15	0.75
1:B:644:ASP:OD2	1:B:646:GLN:HG3	1.87	0.75
1:A:291:LYS:HA	1:A:325:MET:CE	2.16	0.75
1:A:75:ILE:O	1:A:77:THR:HG23	1.87	0.75
1:A:329:ILE:N	1:A:329:ILE:CD1	2.47	0.75
1:B:608:ILE:O	1:B:612:ILE:HG13	1.87	0.74
1:A:218:TYR:O	1:A:258:PRO:HG2	1.86	0.74
1:B:610:ARG:NH2	4:B:921:LAR:H213	2.03	0.74
1:B:718:THR:HA	1:B:727:ILE:CD1	2.16	0.74
1:A:79:TRP:CZ3	1:A:118:LYS:HG2	2.23	0.74
1:A:219:VAL:HB	1:A:307:PRO:O	1.88	0.74
1:A:23:GLY:HA2	1:B:464:ILE:HD13	1.70	0.73
1:B:426:ALA:HB1	1:B:427:PRO:HD2	1.69	0.73
1:B:612:ILE:HG12	1:B:640:TYR:CE2	2.23	0.73
1:A:97:ALA:HB1	1:A:99:GLU:OE1	1.87	0.73
1:B:638:LYS:HG3	1:B:639:SER:N	2.04	0.73
1:A:32:PRO:HB2	1:A:34:ILE:HD13	1.69	0.73
1:A:89:THR:HA	1:A:93:GLU:HB2	1.70	0.73
1:A:217:CYS:HB2	1:A:254:ARG:O	1.88	0.73
1:A:198:TYR:CZ	1:A:248:ILE:HG13	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LYS:C	1:B:593:LEU:H	1.91	0.72
1:B:488:HIS:CE1	1:B:493:GLU:HG2	2.25	0.72
1:A:182:GLY:O	1:A:185:LEU:HB3	1.89	0.71
1:A:286:ASP:O	1:A:289:ILE:HG12	1.90	0.71
1:B:433:SER:O	1:B:434:ILE:HG23	1.90	0.71
1:B:431:PHE:CD2	1:B:493:GLU:HG3	2.26	0.71
1:A:206:ARG:O	1:A:208:ILE:N	2.23	0.71
1:A:78:ASN:OD1	1:A:81:ASP:HB2	1.90	0.71
1:B:683:MET:HE1	1:B:690:ARG:HD3	1.72	0.71
1:B:683:MET:C	1:B:685:CYS:H	1.94	0.71
1:B:642:LEU:HB3	1:B:643:PRO:HD2	1.72	0.70
1:A:164:PRO:HG2	1:A:171:LEU:HB2	1.74	0.70
1:A:348:SER:OG	1:B:464:ILE:HD12	1.92	0.70
1:A:190:MET:CA	1:A:209:VAL:HG21	2.22	0.69
1:B:459:GLN:HG3	1:B:462:ARG:HB2	1.74	0.69
1:B:583:ARG:HA	1:B:586:THR:HB	1.74	0.69
1:B:594:THR:HA	1:B:598:TYR:O	1.91	0.69
1:B:699:MET:HE2	1:B:731:ALA:HB2	1.72	0.69
1:B:607:GLU:OE2	4:B:921:LAR:H191	1.92	0.69
1:B:590:MET:HA	1:B:609:VAL:HG21	1.75	0.69
1:A:182:GLY:HA2	1:A:303:THR:HG21	1.73	0.69
1:B:523:MET:CE	1:B:529:VAL:HG11	2.23	0.69
1:B:627:MET:HA	1:B:655:PHE:HZ	1.57	0.69
1:B:556:GLY:HA3	3:B:880:ATP:O3G	1.92	0.68
1:B:589:LEU:HD23	1:B:609:VAL:HG22	1.75	0.68
1:A:36:GLY:HA2	1:A:67:LEU:HD23	1.74	0.68
1:A:142:LEU:CD2	1:A:165:ILE:HD12	2.23	0.68
1:B:619:VAL:HG21	1:B:709:ILE:HA	1.75	0.68
1:A:89:THR:O	1:A:93:GLU:HB2	1.93	0.68
1:A:291:LYS:HA	1:A:325:MET:HE2	1.75	0.68
1:B:699:MET:O	1:B:735:ARG:HG2	1.94	0.67
1:A:133:TYR:HE1	1:A:135:ALA:HB2	1.59	0.67
1:A:147:ARG:H	1:A:147:ARG:HD2	1.58	0.67
1:A:228:ALA:HA	1:A:231:ALA:CB	2.23	0.67
1:A:37:ARG:O	1:A:65:LEU:HB3	1.94	0.67
1:B:509:PRO:O	1:B:510:LEU:HB2	1.94	0.67
1:B:554:ASP:HA	1:B:700:SER:O	1.94	0.67
1:B:586:THR:HG21	4:B:921:LAR:S1	2.35	0.66
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.77	0.66
1:A:230:ALA:HB2	1:A:236:LEU:CD1	2.23	0.66
1:A:274:ILE:HG22	1:A:313:MET:SD	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:GLY:O	1:B:705:MET:HB2	1.95	0.66
1:B:438:PRO:HD2	1:B:451:ASP:O	1.96	0.66
1:A:242:LEU:CB	1:A:246:GLN:HB2	2.25	0.66
1:B:617:CYS:HB3	1:B:654:ARG:HA	1.77	0.66
1:A:147:ARG:NH2	1:A:330:ILE:HD13	2.10	0.66
1:B:654:ARG:O	1:B:658:PRO:HD2	1.96	0.66
1:A:159:VAL:CG2	1:A:160:THR:N	2.59	0.66
1:B:642:LEU:HD21	1:B:648:ILE:CD1	2.26	0.66
1:B:705:MET:HE2	1:B:736:LYS:H	1.59	0.66
1:B:588:TYR:O	1:B:592:ILE:HG13	1.96	0.65
1:B:691:LYS:HA	1:B:725:MET:HE1	1.77	0.65
1:A:304:THR:O	1:A:335:ARG:NH1	2.29	0.65
1:A:142:LEU:HD23	1:A:165:ILE:HD12	1.78	0.65
1:B:657:CYS:HB3	1:B:658:PRO:HD3	1.79	0.65
1:A:132:MET:HA	1:A:356:TRP:CZ3	2.31	0.65
1:A:98:PRO:O	1:A:129:VAL:HA	1.97	0.65
1:B:705:MET:CE	1:B:736:LYS:H	2.10	0.65
1:A:258:PRO:HG3	1:A:306:TYR:CE2	2.32	0.64
1:A:217:CYS:HB3	1:A:254:ARG:HA	1.79	0.64
1:B:424:ASP:HB2	1:B:740:TRP:HH2	1.62	0.64
1:A:32:PRO:CB	1:A:34:ILE:HD13	2.27	0.64
1:B:585:LEU:CD2	1:B:660:THR:HB	2.28	0.64
1:A:120:THR:OG1	1:A:370:VAL:HG21	1.98	0.64
1:A:219:VAL:HG11	1:A:309:ILE:CA	2.28	0.64
1:A:318:THR:HG22	1:A:327:ILE:HD12	1.79	0.64
1:A:165:ILE:HG23	1:A:169:TYR:C	2.17	0.63
1:A:209:VAL:HA	1:A:212:ILE:CD1	2.18	0.63
1:A:247:VAL:HG23	1:A:247:VAL:O	1.98	0.63
1:A:54:VAL:HG12	1:A:55:GLY:N	2.12	0.63
1:A:76:ILE:HG21	1:A:79:TRP:CZ3	2.33	0.63
1:B:638:LYS:CG	1:B:639:SER:H	2.10	0.63
1:A:160:THR:HG23	1:A:180:LEU:O	1.99	0.63
1:A:282:ILE:HG21	1:A:294:TYR:CE2	2.34	0.63
1:A:317:ILE:O	1:A:319:ALA:N	2.31	0.63
1:A:360:GLN:NE2	1:A:364:GLU:OE2	2.31	0.63
1:B:642:LEU:HB2	1:B:646:GLN:HB2	1.80	0.63
1:B:717:ILE:O	1:B:719:ALA:N	2.32	0.63
1:A:357:ILE:HA	1:A:361:GLU:OE1	1.97	0.63
1:A:275:HIS:ND1	1:A:275:HIS:N	2.46	0.63
1:B:421:PHE:HE1	1:B:428:ARG:HD2	1.64	0.63
1:B:549:THR:OG1	1:B:567:GLU:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG21	1:A:309:ILE:HB	1.81	0.62
1:B:481:ASP:OD1	1:B:481:ASP:N	2.31	0.62
1:B:593:LEU:HD23	1:B:609:VAL:CG2	2.23	0.62
1:A:159:VAL:HG22	1:A:160:THR:N	2.14	0.62
1:A:165:ILE:HG22	1:A:169:TYR:N	2.14	0.62
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.82	0.62
1:B:472:GLU:CG	1:B:477:THR:HG21	2.26	0.62
1:B:667:ILE:HB	1:B:669:MET:HG3	1.81	0.62
1:A:242:LEU:CB	1:A:243:PRO:HD2	2.29	0.62
1:A:292:ASP:O	1:A:295:ALA:N	2.33	0.62
1:B:596:ARG:NH1	1:B:651:GLY:HA3	2.08	0.61
1:B:431:PHE:HZ	1:B:489:THR:OG1	1.83	0.61
1:B:589:LEU:CG	1:B:593:LEU:HD22	2.25	0.61
1:A:182:GLY:CA	1:A:303:THR:HG21	2.31	0.61
1:B:691:LYS:HA	1:B:725:MET:CE	2.31	0.61
1:A:73:HIS:HD2	1:A:158:GLY:O	1.84	0.61
1:A:219:VAL:HG21	1:A:309:ILE:N	2.16	0.61
1:B:602:THR:HG23	1:B:605:GLU:N	2.14	0.61
1:A:132:MET:HG2	1:A:133:TYR:H	1.66	0.61
1:B:549:THR:OG1	1:B:566:TYR:HA	2.01	0.61
1:A:291:LYS:HA	1:A:325:MET:HE1	1.83	0.60
1:B:661:LEU:O	1:B:674:ILE:HG13	2.01	0.60
1:B:662:PHE:CE2	1:B:674:ILE:HD12	2.36	0.60
1:B:520:THR:HA	1:B:532:MET:CE	2.31	0.60
1:A:267:ILE:HB	1:A:269:MET:HG3	1.83	0.60
1:A:150:GLY:O	1:A:165:ILE:N	2.29	0.60
1:B:685:CYS:HB3	1:B:689:ILE:HD11	1.81	0.60
1:A:328:LYS:HA	1:A:329:ILE:HD13	1.83	0.60
1:B:610:ARG:HH22	4:B:921:LAR:H213	1.66	0.60
1:B:762:TYR:HE1	1:B:767:PRO:HB3	1.67	0.60
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.02	0.59
1:A:203:THR:O	1:A:206:ARG:HB3	2.01	0.59
1:A:252:ASN:C	1:A:252:ASN:ND2	2.55	0.59
1:B:642:LEU:HB3	1:B:643:PRO:CD	2.32	0.59
1:A:107:GLU:C	1:A:137:GLN:HE21	2.06	0.59
1:A:225:ASN:O	1:A:229:THR:CB	2.51	0.59
1:A:275:HIS:CB	1:A:316:GLU:HB3	2.33	0.59
1:B:523:MET:HE2	1:B:529:VAL:HG11	1.83	0.59
1:A:142:LEU:CD1	1:A:147:ARG:HB2	2.33	0.59
1:B:578:LEU:HG	1:B:580:LEU:HB3	1.84	0.59
1:A:120:THR:HA	1:A:132:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:O	1:A:208:ILE:HG12	2.02	0.59
1:B:406:THR:O	1:B:501:HIS:CD2	2.56	0.59
1:A:30:VAL:O	1:A:30:VAL:HG13	2.03	0.59
1:B:574:ALA:O	1:B:681:SER:OG	2.21	0.59
1:B:622:ASP:CG	1:B:625:ASN:HB3	2.23	0.59
1:A:274:ILE:HG22	1:A:275:HIS:N	2.17	0.59
1:B:667:ILE:HG22	1:B:667:ILE:O	2.03	0.59
1:A:154:ASP:O	1:A:160:THR:HA	2.02	0.58
1:B:482:MET:O	1:B:485:ILE:HB	2.03	0.58
1:B:705:MET:HE2	1:B:736:LYS:N	2.18	0.58
1:A:136:ILE:HG22	1:A:139:VAL:H	1.69	0.58
1:A:267:ILE:HG22	1:A:267:ILE:O	2.03	0.58
1:A:37:ARG:O	1:A:38:PRO:O	2.22	0.58
1:B:473:HIS:HA	1:B:558:GLY:O	2.03	0.58
1:A:185:LEU:CD2	1:A:306:TYR:OH	2.51	0.58
1:B:416:LEU:HD23	1:B:432:PRO:HA	1.86	0.58
1:A:170:ALA:O	1:A:172:PRO:HD3	2.03	0.58
1:A:190:MET:N	1:A:209:VAL:HG21	2.19	0.58
1:A:242:LEU:CB	1:A:243:PRO:CD	2.82	0.58
1:B:589:LEU:HD12	1:B:592:ILE:CD1	2.30	0.58
1:B:475:ILE:O	1:B:477:THR:HG23	2.04	0.58
1:A:99:GLU:HA	1:A:128:ASN:O	2.04	0.57
1:A:107:GLU:O	1:A:137:GLN:HG3	2.04	0.57
1:A:207:GLU:OE2	4:A:901:LAR:H191	2.04	0.57
1:A:313:MET:O	1:A:317:ILE:HG12	2.03	0.57
1:B:421:PHE:O	1:B:424:ASP:HB2	2.03	0.57
1:A:186:THR:HG23	1:A:209:VAL:HG13	1.85	0.57
1:B:644:ASP:O	1:B:646:GLN:N	2.36	0.57
1:B:643:PRO:C	1:B:645:GLY:H	2.06	0.57
1:A:59:GLN:NE2	1:A:59:GLN:CA	2.64	0.57
1:B:580:LEU:HB2	1:B:669:MET:SD	2.44	0.57
1:B:609:VAL:O	1:B:612:ILE:HB	2.04	0.57
1:A:139:VAL:HG22	1:A:165:ILE:HD13	1.85	0.57
1:B:746:LEU:HD21	1:B:752:PHE:CD1	2.40	0.57
1:A:70:PRO:HA	1:A:78:ASN:HB3	1.86	0.57
1:A:151:ILE:HG23	1:A:297:ASN:OD1	2.04	0.57
1:B:585:LEU:HD11	1:B:661:LEU:CG	2.34	0.56
1:B:619:VAL:HG21	1:B:709:ILE:CA	2.35	0.56
1:B:627:MET:HG3	1:B:652:ASN:HD22	1.69	0.56
1:B:628:ALA:C	1:B:630:ALA:H	2.06	0.56
1:A:142:LEU:HD11	1:A:147:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LYS:C	1:B:593:LEU:N	2.59	0.56
1:B:608:ILE:C	1:B:610:ARG:N	2.56	0.56
1:A:152:VAL:HG12	1:A:153:LEU:N	2.20	0.56
1:B:654:ARG:O	1:B:658:PRO:CD	2.52	0.56
1:B:752:PHE:C	1:B:754:GLN:H	2.08	0.56
1:A:151:ILE:HA	1:A:163:VAL:O	2.06	0.56
1:A:295:ALA:O	1:A:328:LYS:CB	2.54	0.56
1:B:488:HIS:CD2	1:B:492:ASN:HD21	2.22	0.56
1:B:762:TYR:CE1	1:B:767:PRO:HB3	2.40	0.56
1:A:219:VAL:HG21	1:A:309:ILE:CA	2.36	0.56
1:B:410:CYS:HB3	1:B:505:LEU:HD23	1.88	0.56
1:B:437:ARG:C	1:B:465:LEU:HD22	2.26	0.56
1:B:626:GLU:C	1:B:628:ALA:N	2.59	0.56
1:B:644:ASP:OD2	1:B:646:GLN:NE2	2.34	0.56
1:A:193:LEU:O	1:A:198:TYR:HD1	1.89	0.55
1:A:223:PHE:O	1:A:227:MET:HB2	2.05	0.55
1:B:443:VAL:O	1:B:443:VAL:HG12	2.06	0.55
1:B:694:TYR:CB	1:B:725:MET:HE3	2.35	0.55
1:A:183:ARG:O	1:A:186:THR:N	2.39	0.55
1:A:275:HIS:HB3	1:A:316:GLU:HB3	1.89	0.55
1:B:542:LEU:O	1:B:545:SER:OG	2.16	0.55
1:B:409:VAL:HG21	1:B:744:SER:HA	1.88	0.55
1:A:274:ILE:CG2	1:A:313:MET:SD	2.95	0.55
1:A:359:LYS:O	1:A:362:TYR:HB3	2.06	0.55
1:B:438:PRO:HA	1:B:465:LEU:HD23	1.88	0.55
1:B:581:ALA:O	1:B:585:LEU:HG	2.07	0.55
1:A:155:SER:OG	1:A:160:THR:CG2	2.55	0.55
1:B:454:VAL:HG12	1:B:455:GLY:N	2.21	0.55
1:A:178:LEU:HD12	1:A:179:ASP:N	2.21	0.55
1:A:72:GLU:HB2	1:A:77:THR:HG21	1.89	0.55
1:A:186:THR:CG2	1:A:209:VAL:HG13	2.37	0.55
1:A:218:TYR:O	1:A:255:PHE:HA	2.06	0.55
1:A:258:PRO:O	1:A:260:THR:N	2.40	0.55
1:A:11:ASP:CG	1:A:106:THR:HG21	2.28	0.54
1:A:154:ASP:HA	1:A:300:SER:O	2.07	0.54
1:A:300:SER:O	1:A:304:THR:HG21	2.06	0.54
1:A:314:GLN:OE1	1:A:329:ILE:HD12	2.07	0.54
1:B:416:LEU:CB	1:B:418:LYS:HE2	2.36	0.54
1:B:548:THR:O	1:B:568:GLY:N	2.38	0.54
1:B:565:ILE:HG23	1:B:569:TYR:C	2.27	0.54
1:B:717:ILE:O	1:B:718:THR:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:O	1:A:172:PRO:CD	2.55	0.54
1:B:606:ARG:O	1:B:608:ILE:N	2.39	0.54
1:A:306:TYR:CZ	3:A:380:ATP:H2	2.26	0.54
1:B:626:GLU:C	1:B:628:ALA:H	2.09	0.54
1:A:147:ARG:CZ	1:A:330:ILE:HD13	2.37	0.54
1:A:282:ILE:HD12	1:A:282:ILE:H	1.71	0.54
1:B:414:SER:CA	1:B:471:ILE:HG22	2.35	0.54
1:B:595:GLU:C	1:B:597:GLY:H	2.11	0.54
1:B:722:PRO:C	1:B:724:THR:H	2.11	0.54
1:B:618:TYR:H	1:B:618:TYR:HD2	1.54	0.54
1:A:32:PRO:HB2	1:A:34:ILE:CD1	2.37	0.54
1:B:627:MET:HA	1:B:655:PHE:CZ	2.40	0.54
1:A:177:ARG:CZ	1:A:179:ASP:OD1	2.56	0.54
1:B:578:LEU:HG	1:B:580:LEU:H	1.73	0.54
1:B:758:THR:HG23	1:B:761:GLU:OE2	2.08	0.54
1:A:79:TRP:CH2	1:A:118:LYS:HG2	2.43	0.53
1:A:206:ARG:HA	1:A:209:VAL:HG12	1.89	0.53
1:B:647:VAL:O	1:B:648:ILE:HG23	2.07	0.53
1:B:733:PRO:HD2	1:B:734:GLU:OE1	2.07	0.53
1:A:314:GLN:OE1	1:A:329:ILE:CD1	2.56	0.53
1:B:699:MET:HE3	1:B:731:ALA:HB2	1.86	0.53
1:A:89:THR:CA	1:A:93:GLU:HB2	2.37	0.53
1:B:459:GLN:OE1	4:B:921:LAR:H223	2.08	0.53
1:B:507:GLU:O	1:B:537:GLN:HG3	2.09	0.53
1:A:219:VAL:HG21	1:A:309:ILE:CB	2.39	0.53
1:B:523:MET:HE3	1:B:529:VAL:HG11	1.90	0.53
1:B:565:ILE:HG23	1:B:569:TYR:N	2.24	0.53
1:B:675:HIS:CG	1:B:676:GLU:N	2.76	0.53
1:A:133:TYR:CE1	1:A:135:ALA:HB2	2.41	0.53
1:A:155:SER:OG	1:A:160:THR:HG21	2.08	0.53
1:A:321:ALA:HB1	1:A:322:PRO:HD2	1.91	0.53
1:B:565:ILE:CG2	1:B:569:TYR:N	2.72	0.53
1:B:675:HIS:CG	1:B:676:GLU:H	2.26	0.53
1:A:59:GLN:O	1:A:62:ARG:HD3	2.09	0.53
1:A:20:GLY:HA3	1:A:340:TRP:CZ2	2.44	0.53
1:B:520:THR:HG23	1:B:532:MET:SD	2.49	0.53
1:A:122:ILE:O	1:A:123:MET:C	2.47	0.53
1:A:262:PHE:CE1	1:A:312:ARG:HG3	2.44	0.53
1:B:627:MET:CE	1:B:652:ASN:ND2	2.72	0.53
1:B:745:ILE:HG22	1:B:746:LEU:N	2.23	0.53
1:A:11:ASP:HA	1:A:106:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:MET:HG2	1:B:533:TYR:H	1.67	0.52
1:A:357:ILE:CD1	1:A:370:VAL:HA	2.39	0.52
1:B:618:TYR:N	1:B:618:TYR:CD2	2.77	0.52
1:A:73:HIS:CD2	1:A:158:GLY:O	2.62	0.52
1:B:493:GLU:HA	1:B:493:GLU:OE1	2.09	0.52
1:B:718:THR:HG22	1:B:727:ILE:HD12	1.91	0.52
1:A:193:LEU:O	1:A:198:TYR:CD1	2.62	0.52
1:A:309:ILE:HG23	1:A:310:ALA:N	2.25	0.52
1:A:317:ILE:O	1:A:320:LEU:N	2.31	0.52
1:B:454:VAL:HB	1:B:488:HIS:CD2	2.45	0.52
1:B:650:ILE:CG2	1:B:654:ARG:HD2	2.38	0.52
1:A:257:CYS:HB3	1:A:258:PRO:CD	2.36	0.52
1:A:317:ILE:O	1:A:318:THR:C	2.48	0.52
1:A:54:VAL:CG1	1:A:55:GLY:N	2.73	0.52
1:B:638:LYS:O	1:B:650:ILE:N	2.34	0.52
1:B:682:ILE:HG23	1:B:693:LEU:HB2	1.92	0.52
1:A:109:PRO:HB2	1:A:161:HIS:CD2	2.45	0.52
1:B:507:GLU:O	1:B:537:GLN:NE2	2.43	0.52
1:B:635:SER:OG	1:B:636:LEU:N	2.43	0.52
1:A:260:THR:CG2	1:A:267:ILE:HG12	2.40	0.52
1:A:91:TYR:CE2	1:A:98:PRO:HD2	2.45	0.51
1:A:241:GLU:CA	1:A:246:GLN:O	2.52	0.51
1:B:587:ASP:OD2	1:B:606:ARG:HD2	2.10	0.51
1:A:210:ARG:O	1:A:213:LYS:HB3	2.09	0.51
1:B:433:SER:O	1:B:434:ILE:CG2	2.58	0.51
1:B:588:TYR:HB2	1:B:667:ILE:HD11	1.91	0.51
1:A:107:GLU:HG2	1:A:108:ALA:N	2.23	0.51
1:B:639:SER:HA	1:B:649:THR:HA	1.92	0.51
1:A:142:LEU:HD22	1:A:165:ILE:HD12	1.92	0.51
1:A:197:GLY:C	1:A:198:TYR:CD1	2.84	0.51
1:B:551:ILE:HA	1:B:564:PRO:HA	1.93	0.51
1:B:613:LYS:CA	1:B:617:CYS:SG	2.98	0.51
1:A:322:PRO:HG2	1:A:325:MET:HG2	1.92	0.51
1:A:349:LEU:O	1:A:352:PHE:HB3	2.11	0.51
1:A:177:ARG:O	1:A:177:ARG:HG2	2.10	0.51
1:B:585:LEU:HD21	1:B:660:THR:HB	1.91	0.51
1:A:222:ASP:O	1:A:226:GLU:HB3	2.11	0.51
1:A:299:MET:O	1:A:335:ARG:HG2	2.11	0.51
1:B:595:GLU:C	1:B:597:GLY:N	2.64	0.51
1:B:618:TYR:CE2	1:B:655:PHE:HB3	2.46	0.51
1:A:190:MET:CB	1:A:209:VAL:HG11	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:THR:O	1:A:101:HIS:HD2	1.93	0.51
1:A:36:GLY:HA3	1:A:67:LEU:HD23	1.92	0.51
1:A:182:GLY:HA2	1:A:303:THR:CG2	2.39	0.51
1:A:285:CYS:O	1:A:286:ASP:C	2.49	0.51
1:B:617:CYS:HB2	1:B:654:ARG:O	2.11	0.51
1:A:302:GLY:O	1:A:305:MET:CB	2.58	0.50
1:B:618:TYR:HD2	1:B:618:TYR:N	2.08	0.50
1:A:12:ASN:ND2	1:A:12:ASN:H	2.08	0.50
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.93	0.50
1:A:311:ASP:O	1:A:312:ARG:C	2.49	0.50
1:B:585:LEU:HD11	1:B:661:LEU:CD2	2.41	0.50
1:A:21:PHE:HE1	1:A:28:ARG:HD3	1.76	0.50
1:A:206:ARG:O	1:A:209:VAL:HG12	2.12	0.50
1:A:210:ARG:HG3	4:A:901:LAR:O5	2.11	0.50
1:A:9:VAL:O	1:A:340:TRP:NE1	2.39	0.50
1:A:151:ILE:HG23	1:A:151:ILE:O	2.11	0.50
1:A:88:HIS:O	1:A:92:ASN:OD1	2.30	0.50
1:B:627:MET:HE2	1:B:652:ASN:HD21	1.76	0.50
1:A:165:ILE:CG2	1:A:169:TYR:C	2.79	0.50
1:A:255:PHE:O	1:A:259:GLU:HB2	2.12	0.50
1:B:424:ASP:CB	1:B:740:TRP:HH2	2.24	0.50
1:B:520:THR:HG21	1:B:770:VAL:CG2	2.42	0.50
1:B:702:GLY:HA3	3:B:880:ATP:O4'	2.12	0.49
1:B:589:LEU:O	1:B:593:LEU:CB	2.49	0.49
1:B:695:ALA:O	1:B:728:LYS:HB3	2.12	0.49
1:A:190:MET:HB3	1:A:209:VAL:HG21	1.94	0.49
1:A:76:ILE:HG21	1:A:79:TRP:CE3	2.46	0.49
1:A:79:TRP:CE3	1:A:118:LYS:HG2	2.47	0.49
1:A:155:SER:HA	1:A:160:THR:HB	1.94	0.49
1:B:751:THR:O	1:B:754:GLN:HG2	2.12	0.49
1:A:123:MET:HB3	1:A:129:VAL:HG21	1.94	0.49
1:A:183:ARG:O	1:A:184:ASP:C	2.51	0.49
1:A:264:PRO:HG2	1:A:271:SER:O	2.12	0.49
4:A:901:LAR:H42	4:A:901:LAR:O2	2.12	0.49
1:A:118:LYS:O	1:A:119:MET:C	2.48	0.49
1:A:142:LEU:HD11	1:A:147:ARG:CB	2.42	0.49
1:B:608:ILE:C	1:B:610:ARG:H	2.16	0.49
1:A:164:PRO:HG2	1:A:164:PRO:O	2.12	0.49
1:B:447:MET:HA	1:B:447:MET:CE	2.43	0.49
1:A:17:VAL:O	1:A:30:VAL:HA	2.12	0.49
1:A:313:MET:O	1:A:314:GLN:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HG13	1:A:65:LEU:HG	1.94	0.49
1:B:476:ILE:HD13	1:B:482:MET:HG2	1.94	0.49
1:A:114:ALA:C	1:A:116:ARG:N	2.66	0.49
1:B:717:ILE:C	1:B:719:ALA:N	2.65	0.49
1:B:758:THR:OG1	1:B:761:GLU:HG3	2.13	0.49
1:B:490:PHE:CE1	1:B:527:PHE:CD1	3.01	0.48
1:A:149:THR:OG1	1:A:167:GLU:CA	2.60	0.48
1:A:305:MET:HE2	1:A:336:LYS:H	1.78	0.48
1:B:520:THR:OG1	1:B:770:VAL:HG21	2.13	0.48
1:B:462:ARG:HA	1:B:465:LEU:HB2	1.94	0.48
1:B:528:ASN:N	1:B:528:ASN:HD22	2.11	0.48
1:B:590:MET:CA	1:B:609:VAL:HG21	2.42	0.48
1:A:14:SER:HA	1:A:71:ILE:HG22	1.96	0.48
1:B:766:GLY:C	1:B:768:SER:H	2.15	0.48
1:A:322:PRO:C	1:A:324:THR:H	2.17	0.48
1:B:532:MET:HE2	1:B:534:VAL:CG2	2.44	0.48
1:A:189:LEU:HD23	1:A:213:LYS:HB2	1.95	0.48
1:B:533:TYR:HE1	1:B:535:ALA:HB2	1.79	0.48
1:B:585:LEU:HD22	1:B:660:THR:HB	1.94	0.48
1:B:489:THR:HA	1:B:493:GLU:HB2	1.96	0.48
1:A:190:MET:HA	1:A:209:VAL:HG21	1.94	0.48
1:A:258:PRO:HG3	1:A:306:TYR:CD2	2.49	0.48
1:B:469:TYR:OH	4:B:921:LAR:H181	2.14	0.48
1:B:523:MET:HE3	1:B:529:VAL:CG1	2.43	0.48
1:B:652:ASN:C	1:B:654:ARG:H	2.17	0.48
1:A:208:ILE:O	1:A:211:ASP:N	2.47	0.48
1:B:628:ALA:C	1:B:630:ALA:N	2.67	0.48
1:A:185:LEU:HD11	1:A:258:PRO:HA	1.96	0.47
1:B:426:ALA:HB1	1:B:427:PRO:CD	2.43	0.47
1:B:459:GLN:OE1	4:B:921:LAR:C9	2.62	0.47
1:B:478:ASN:ND2	1:B:481:ASP:OD1	2.47	0.47
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.55	0.47
1:B:606:ARG:C	1:B:608:ILE:N	2.67	0.47
1:B:643:PRO:C	1:B:645:GLY:N	2.68	0.47
1:A:190:MET:CB	1:A:209:VAL:HG21	2.44	0.47
1:A:101:HIS:O	1:A:130:PRO:HD2	2.15	0.47
1:A:132:MET:CG	1:A:133:TYR:N	2.73	0.47
1:A:316:GLU:OE1	1:A:316:GLU:HA	2.11	0.47
1:B:498:PRO:HB2	1:B:527:PHE:HB3	1.96	0.47
1:B:606:ARG:HA	1:B:609:VAL:HG12	1.96	0.47
1:A:206:ARG:C	1:A:208:ILE:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:O	1:A:282:ILE:C	2.54	0.47
1:B:554:ASP:O	1:B:560:THR:HA	2.14	0.47
1:B:566:TYR:CD2	1:B:567:GLU:N	2.83	0.47
1:A:188:TYR:O	1:A:191:LYS:HB3	2.15	0.47
1:B:644:ASP:C	1:B:646:GLN:H	2.18	0.47
1:A:171:LEU:O	1:A:172:PRO:C	2.52	0.47
1:B:694:TYR:HB2	1:B:725:MET:HE3	1.96	0.47
1:B:502:PRO:HA	1:B:531:ALA:O	2.16	0.46
1:B:593:LEU:HD12	1:B:593:LEU:HA	1.70	0.46
1:A:11:ASP:HA	1:A:106:THR:HG23	1.96	0.46
1:A:59:GLN:HE21	1:A:59:GLN:CA	1.99	0.46
1:A:132:MET:HA	1:A:356:TRP:HZ3	1.76	0.46
1:B:451:ASP:HB3	1:B:453:TYR:CE1	2.50	0.46
1:A:9:VAL:HG12	1:A:340:TRP:CD1	2.51	0.46
1:A:208:ILE:C	1:A:210:ARG:N	2.66	0.46
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.97	0.46
1:B:507:GLU:C	1:B:537:GLN:NE2	2.68	0.46
1:B:566:TYR:HD2	1:B:567:GLU:N	2.14	0.46
1:B:479:TRP:HZ2	1:B:515:ASN:ND2	2.13	0.46
1:B:524:PHE:CE2	1:B:759:LYS:HA	2.50	0.46
1:B:542:LEU:CD1	1:B:547:ARG:HB2	2.45	0.46
1:B:722:PRO:C	1:B:724:THR:N	2.69	0.46
1:B:542:LEU:HD11	1:B:547:ARG:HB2	1.97	0.46
1:B:753:GLN:HA	1:B:756:TRP:HD1	1.80	0.46
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.49	0.46
1:A:152:VAL:CG1	1:A:153:LEU:N	2.77	0.46
1:A:219:VAL:CG1	1:A:309:ILE:HA	2.39	0.46
1:A:350:SER:O	1:A:353:GLN:CB	2.64	0.46
1:B:606:ARG:C	1:B:608:ILE:H	2.19	0.46
1:B:702:GLY:O	1:B:705:MET:CB	2.63	0.46
1:B:714:GLN:HE22	1:B:727:ILE:HG22	1.81	0.46
1:A:155:SER:HA	1:A:160:THR:CB	2.46	0.46
1:A:210:ARG:HH12	4:A:901:LAR:H41	1.81	0.46
1:B:516:ARG:HA	1:B:519:MET:HB2	1.97	0.46
1:B:551:ILE:HD13	1:B:682:ILE:CD1	2.46	0.46
1:A:183:ARG:O	1:A:185:LEU:N	2.49	0.46
1:A:265:SER:O	1:A:267:ILE:N	2.49	0.46
1:B:541:SER:OG	1:B:739:VAL:HG22	2.16	0.46
1:B:587:ASP:HA	1:B:590:MET:HE2	1.98	0.46
1:B:588:TYR:HB2	1:B:667:ILE:CD1	2.45	0.46
1:A:88:HIS:CE1	1:A:93:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:THR:HG1	1:B:567:GLU:H	1.58	0.45
1:B:616:LEU:O	1:B:617:CYS:C	2.55	0.45
1:A:124:PHE:CE2	1:A:359:LYS:HA	2.51	0.45
1:A:346:LEU:HD21	1:A:352:PHE:CE1	2.52	0.45
1:B:438:PRO:HG3	1:B:451:ASP:HB2	1.99	0.45
1:B:547:ARG:H	1:B:547:ARG:HD2	1.80	0.45
1:A:90:PHE:O	1:A:95:ARG:N	2.48	0.45
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.16	0.45
1:B:689:ILE:HG13	1:B:690:ARG:N	2.32	0.45
1:B:753:GLN:HA	1:B:756:TRP:CD1	2.52	0.45
1:B:650:ILE:HG21	1:B:654:ARG:HD2	1.97	0.45
1:A:261:LEU:HB3	1:A:274:ILE:HD11	1.97	0.45
1:B:507:GLU:HG2	1:B:508:ALA:N	2.32	0.45
1:B:516:ARG:O	1:B:519:MET:HB3	2.17	0.45
1:A:206:ARG:O	1:A:207:GLU:C	2.55	0.45
1:A:217:CYS:CB	1:A:254:ARG:HA	2.45	0.45
1:B:438:PRO:CD	1:B:451:ASP:O	2.64	0.45
1:B:444:MET:HE2	1:B:447:MET:HG3	1.97	0.45
1:B:598:TYR:HE2	1:B:648:ILE:CG2	2.29	0.45
1:B:752:PHE:O	1:B:754:GLN:N	2.49	0.45
1:B:432:PRO:HB2	4:B:921:LAR:H121	1.97	0.45
1:B:589:LEU:HD23	1:B:609:VAL:O	2.16	0.45
1:B:497:ALA:HB1	1:B:499:GLU:OE1	2.17	0.45
1:B:664:PRO:HB2	1:B:669:MET:HB2	1.98	0.45
1:A:94:LEU:O	1:A:96:VAL:HG13	2.17	0.45
1:A:190:MET:SD	1:A:206:ARG:HA	2.57	0.45
1:B:674:ILE:HG22	1:B:675:HIS:H	1.81	0.45
1:A:114:ALA:O	1:A:116:ARG:N	2.50	0.45
1:A:166:TYR:O	1:A:167:GLU:C	2.55	0.45
1:B:682:ILE:HG22	1:B:682:ILE:O	2.16	0.45
1:A:147:ARG:H	1:A:147:ARG:CD	2.27	0.44
1:A:164:PRO:O	1:A:164:PRO:CG	2.65	0.44
1:A:178:LEU:HD12	1:A:178:LEU:C	2.37	0.44
1:A:272:ALA:HB1	1:A:276:GLU:OE1	2.17	0.44
1:B:578:LEU:CG	1:B:580:LEU:HB3	2.47	0.44
1:B:625:ASN:OD1	1:B:625:ASN:O	2.35	0.44
1:A:36:GLY:CA	1:A:67:LEU:CD2	2.93	0.44
1:A:102:PRO:HA	1:A:131:ALA:O	2.16	0.44
1:B:411:ASP:HB3	1:B:418:LYS:HB2	1.99	0.44
1:B:414:SER:CA	1:B:471:ILE:CG2	2.91	0.44
1:B:524:PHE:O	1:B:528:ASN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:TYR:CD1	1:B:534:VAL:N	2.86	0.44
1:B:617:CYS:HA	1:B:654:ARG:CG	2.41	0.44
1:B:506:THR:HB	1:B:537:GLN:HG2	1.99	0.44
1:A:265:SER:OG	1:A:266:PHE:N	2.51	0.44
1:B:444:MET:HG2	1:B:447:MET:HG2	1.99	0.44
1:A:153:LEU:HD12	1:A:161:HIS:O	2.18	0.44
1:A:213:LYS:O	1:A:214:GLU:C	2.56	0.44
1:B:536:ILE:O	1:B:539:VAL:HB	2.17	0.44
1:B:675:HIS:N	1:B:675:HIS:ND1	2.65	0.44
1:B:711:ASP:O	1:B:714:GLN:HB3	2.17	0.44
1:B:735:ARG:O	1:B:736:LYS:C	2.54	0.44
1:B:590:MET:HG2	1:B:609:VAL:CG1	2.30	0.44
1:B:745:ILE:O	1:B:746:LEU:C	2.55	0.44
1:B:432:PRO:HB3	4:B:921:LAR:H141	2.00	0.44
1:B:673:GLY:HA3	1:B:675:HIS:CE1	2.53	0.44
1:A:16:LEU:O	1:A:18:LYS:HE2	2.18	0.43
1:A:165:ILE:HG23	1:A:170:ALA:CA	2.47	0.43
1:A:279:TYR:CE1	1:A:283:MET:HE2	2.52	0.43
1:A:279:TYR:O	1:A:280:ASN:C	2.56	0.43
1:B:542:LEU:HD11	1:B:547:ARG:CB	2.48	0.43
1:A:181:ALA:O	1:A:185:LEU:HB2	2.18	0.43
1:A:303:THR:C	1:A:305:MET:H	2.20	0.43
1:A:36:GLY:HA3	1:A:67:LEU:CD2	2.47	0.43
1:A:305:MET:HE1	1:A:335:ARG:HB2	1.99	0.43
1:A:185:LEU:HD21	1:A:306:TYR:OH	2.16	0.43
1:A:348:SER:OG	1:B:464:ILE:CD1	2.63	0.43
1:B:565:ILE:CA	1:B:569:TYR:O	2.57	0.43
1:B:660:THR:CG2	1:B:667:ILE:HG12	2.48	0.43
1:A:143:TYR:CE2	1:A:346:LEU:HD12	2.53	0.43
1:A:264:PRO:O	1:A:265:SER:C	2.57	0.43
1:A:366:GLY:O	1:A:369:ILE:CG2	2.49	0.43
1:B:580:LEU:HD12	1:B:581:ALA:N	2.33	0.43
1:B:608:ILE:O	1:B:610:ARG:N	2.51	0.43
1:A:282:ILE:O	1:A:285:CYS:HB2	2.19	0.43
1:B:623:PHE:CE1	1:B:659:GLU:HG2	2.54	0.43
1:A:171:LEU:HA	1:A:172:PRO:HD2	1.62	0.43
1:A:16:LEU:O	1:A:18:LYS:CE	2.67	0.43
1:A:151:ILE:CG2	1:A:297:ASN:OD1	2.67	0.43
1:A:206:ARG:HG2	4:A:901:LAR:S1	2.59	0.43
1:B:504:LEU:CD1	1:B:533:TYR:HD1	2.31	0.43
1:B:627:MET:HE3	1:B:652:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:OD1	1:A:92:ASN:C	2.56	0.43
1:B:627:MET:HG3	1:B:652:ASN:ND2	2.33	0.42
1:B:666:PHE:N	1:B:666:PHE:CD2	2.87	0.42
1:A:37:ARG:C	1:A:65:LEU:HD22	2.39	0.42
1:A:107:GLU:HB2	1:A:134:VAL:HG12	2.00	0.42
1:A:120:THR:O	1:A:121:GLN:C	2.57	0.42
1:B:604:ALA:O	1:B:608:ILE:CG1	2.62	0.42
1:B:606:ARG:O	1:B:609:VAL:HG12	2.18	0.42
1:A:119:MET:O	1:A:122:ILE:HB	2.19	0.42
1:A:186:THR:O	1:A:189:LEU:N	2.52	0.42
1:A:292:ASP:O	1:A:293:LEU:C	2.57	0.42
1:A:341:ILE:O	1:A:345:ILE:HG13	2.19	0.42
1:B:412:ASN:ND2	1:B:486:TRP:NE1	2.53	0.42
1:B:585:LEU:HD13	1:B:658:PRO:HA	2.01	0.42
1:B:444:MET:CE	1:B:447:MET:HG2	2.48	0.42
1:A:107:GLU:OE2	1:A:116:ARG:HD3	2.19	0.42
1:B:507:GLU:HG2	1:B:508:ALA:H	1.83	0.42
1:B:690:ARG:O	1:B:691:LYS:C	2.57	0.42
1:A:88:HIS:CE1	1:A:93:GLU:CG	3.02	0.42
1:A:104:LEU:HD11	1:A:133:TYR:HD1	1.83	0.42
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.79	0.42
1:B:454:VAL:O	1:B:455:GLY:O	2.37	0.42
1:A:242:LEU:CB	1:A:246:GLN:NE2	2.83	0.42
1:B:644:ASP:C	1:B:646:GLN:N	2.73	0.42
1:B:664:PRO:O	1:B:669:MET:HB2	2.20	0.42
1:B:553:LEU:HB3	1:B:699:MET:HG2	2.02	0.42
1:B:652:ASN:HB2	1:B:655:PHE:CZ	2.54	0.42
1:A:149:THR:HG23	1:A:166:TYR:HA	2.01	0.42
1:A:198:TYR:CE2	1:A:248:ILE:HD12	2.55	0.42
1:A:218:TYR:OH	1:A:226:GLU:OE2	2.37	0.42
1:A:352:PHE:O	1:A:354:GLN:N	2.52	0.42
1:A:104:LEU:HA	1:A:104:LEU:HD12	1.61	0.42
1:A:166:TYR:HB2	1:A:171:LEU:HD11	2.02	0.42
1:A:287:ILE:H	1:A:287:ILE:HG22	1.49	0.42
1:B:566:TYR:CD2	1:B:566:TYR:C	2.93	0.41
1:B:627:MET:CE	1:B:652:ASN:HD21	2.32	0.41
1:B:699:MET:O	1:B:735:ARG:CG	2.66	0.41
1:A:247:VAL:O	1:A:248:ILE:C	2.58	0.41
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.82	0.41
1:B:717:ILE:O	1:B:720:LEU:N	2.44	0.41
1:A:110:LEU:N	5:A:1017:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ARG:HD3	1:B:606:ARG:NH2	2.35	0.41
1:B:683:MET:HE1	1:B:690:ARG:CD	2.46	0.41
1:B:706:TYR:CZ	3:B:880:ATP:H2	2.38	0.41
1:B:642:LEU:CB	1:B:643:PRO:CD	2.97	0.41
1:A:185:LEU:HD21	1:A:306:TYR:CZ	2.56	0.41
1:A:346:LEU:C	1:A:346:LEU:HD23	2.41	0.41
1:B:588:TYR:CZ	1:B:592:ILE:HG12	2.56	0.41
1:B:610:ARG:C	1:B:612:ILE:N	2.73	0.41
1:A:9:VAL:HG22	1:A:104:LEU:HB3	2.03	0.41
1:A:183:ARG:C	1:A:185:LEU:N	2.72	0.41
1:B:459:GLN:HG3	1:B:462:ARG:CB	2.47	0.41
1:B:544:ALA:HB2	1:B:742:GLY:CA	2.51	0.41
1:B:589:LEU:HD23	1:B:609:VAL:CG2	2.48	0.41
1:B:589:LEU:HA	1:B:592:ILE:HD11	2.02	0.41
1:B:647:VAL:HG12	1:B:648:ILE:N	2.36	0.41
1:B:690:ARG:C	1:B:692:ASP:N	2.72	0.41
1:A:101:HIS:HA	1:A:102:PRO:HD3	1.90	0.41
1:A:108:ALA:HA	1:A:109:PRO:HD3	1.92	0.41
1:A:309:ILE:CG2	1:A:310:ALA:N	2.83	0.41
1:A:352:PHE:O	1:A:355:MET:HB2	2.21	0.41
1:B:697:ASN:HD22	1:B:698:VAL:N	2.19	0.41
1:A:11:ASP:OD2	1:A:106:THR:HG21	2.21	0.41
1:A:18:LYS:HD2	1:A:18:LYS:N	2.35	0.41
1:A:114:ALA:C	1:A:116:ARG:H	2.24	0.41
1:A:219:VAL:CG2	1:A:309:ILE:HB	2.48	0.41
1:A:242:LEU:N	1:A:246:GLN:O	2.50	0.41
1:B:431:PHE:CE2	1:B:493:GLU:HG3	2.56	0.41
1:B:507:GLU:O	1:B:537:GLN:CG	2.68	0.41
1:B:566:TYR:N	1:B:569:TYR:O	2.50	0.41
1:B:587:ASP:OD1	1:B:606:ARG:NH1	2.53	0.41
1:B:682:ILE:HG21	1:B:694:TYR:CE2	2.55	0.41
1:A:17:VAL:HG12	1:A:18:LYS:N	2.36	0.41
1:A:111:ASN:HD21	1:A:115:ASN:HB3	1.85	0.41
1:A:123:MET:O	1:A:127:PHE:HB2	2.21	0.41
1:A:187:ASP:HA	1:A:190:MET:HG2	2.03	0.41
1:B:741:ILE:O	1:B:742:GLY:C	2.59	0.41
1:A:123:MET:HB3	1:A:129:VAL:CG2	2.52	0.40
1:A:362:TYR:O	1:A:365:ALA:O	2.39	0.40
1:A:132:MET:C	1:A:356:TRP:CE3	2.94	0.40
1:A:289:ILE:O	1:A:290:ARG:C	2.60	0.40
1:A:351:THR:HG21	1:B:448:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HB3	4:A:901:LAR:H121	2.02	0.40
1:A:54:VAL:CG1	1:A:55:GLY:H	2.35	0.40
1:A:303:THR:O	1:A:306:TYR:HD1	2.04	0.40
1:B:461:LYS:O	1:B:465:LEU:HG	2.22	0.40
1:B:522:ILE:O	1:B:523:MET:C	2.59	0.40
1:B:532:MET:CG	1:B:533:TYR:N	2.59	0.40
4:B:921:LAR:O2	4:B:921:LAR:H42	2.22	0.40
1:A:78:ASN:OD1	1:A:81:ASP:CB	2.66	0.40
1:B:408:LEU:CD1	1:B:501:HIS:HB3	2.51	0.40
1:B:414:SER:HB2	3:B:880:ATP:O2G	2.21	0.40
1:B:643:PRO:O	1:B:645:GLY:N	2.41	0.40
1:A:38:PRO:HA	1:A:65:LEU:CD2	2.40	0.40
1:A:224:GLU:O	1:A:227:MET:HB3	2.21	0.40
1:A:230:ALA:CB	1:A:236:LEU:HB2	2.52	0.40
1:A:258:PRO:C	1:A:260:THR:N	2.73	0.40
1:B:520:THR:HG21	1:B:770:VAL:HG22	2.04	0.40
1:B:553:LEU:HD21	1:B:674:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	359/377 (95%)	249 (69%)	80 (22%)	30 (8%)	1 1
1	B	369/377 (98%)	270 (73%)	67 (18%)	32 (9%)	1 1
All	All	728/754 (97%)	519 (71%)	147 (20%)	62 (8%)	1 1

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	PRO

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Mol	Chain	Res	Type
1	A	90	PHE
1	A	207	GLU
1	A	274	ILE
1	A	318	THR
1	B	455	GLY
1	B	674	ILE
1	B	684	LYS
1	B	687	ILE
1	A	30	VAL
1	A	53	TYR
1	A	91	TYR
1	A	122	ILE
1	A	171	LEU
1	A	217	CYS
1	A	242	LEU
1	A	246	GLN
1	A	253	GLU
1	A	254	ARG
1	A	259	GLU
1	A	266	PHE
1	A	317	ILE
1	B	405	THR
1	B	454	VAL
1	B	607	GLU
1	B	617	CYS
1	B	623	PHE
1	B	633	SER
1	B	636	LEU
1	B	645	GLY
1	B	646	GLN
1	B	686	ASP
1	B	718	THR
1	B	735	ARG
1	B	753	GLN
1	A	172	PRO
1	A	179	ASP
1	A	190	MET
1	A	206	ARG
1	A	235	SER
1	A	251	GLY
1	B	637	GLU
1	B	688	ASP

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Mol	Chain	Res	Type
1	B	723	SER
1	A	115	ASN
1	A	124	PHE
1	A	323	SER
1	A	350	SER
1	A	353	GLN
1	B	462	ARG
1	B	590	MET
1	B	653	GLU
1	B	676	GLU
1	B	716	GLU
1	B	440	HIS
1	B	448	GLY
1	B	544	ALA
1	B	666	PHE
1	B	710	ALA
1	A	201	VAL
1	B	717	ILE
1	B	745	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 X-ray entries followed by that with respect to entries of similar resolution.

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	276/320 (86%)	254 (92%)	22 (8%)	12	31
1	B	283/320 (88%)	259 (92%)	24 (8%)	10	28
All	All	559/640 (87%)	513 (92%)	46 (8%)	11	29

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	24	ASP
1	A	34	ILE
1	A	59	GLN

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Mol	Chain	Res	Type
1	A	118	LYS
1	A	121	GLN
1	A	125	GLU
1	A	132	MET
1	A	141	SER
1	A	148	THR
1	A	179	ASP
1	A	206	ARG
1	A	218	TYR
1	A	248	ILE
1	A	252	ASN
1	A	281	SER
1	A	299	MET
1	A	309	ILE
1	A	316	GLU
1	A	326	LYS
1	A	329	ILE
1	A	355	MET
1	B	418	LYS
1	B	447	MET
1	B	471	ILE
1	B	478	ASN
1	B	481	ASP
1	B	528	ASN
1	B	532	MET
1	B	548	THR
1	B	553	LEU
1	B	566	TYR
1	B	596	ARG
1	B	598	TYR
1	B	606	ARG
1	B	618	TYR
1	B	621	LEU
1	B	633	SER
1	B	634	SER
1	B	644	ASP
1	B	652	ASN
1	B	681	SER
1	B	697	ASN
1	B	749	LEU
1	B	755	MET
1	B	772	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	73	HIS
1	A	87	HIS
1	A	88	HIS
1	A	101	HIS
1	A	111	ASN
1	A	128	ASN
1	A	137	GLN
1	A	161	HIS
1	A	246	GLN
1	A	252	ASN
1	B	412	ASN
1	B	473	HIS
1	B	478	ASN
1	B	487	HIS
1	B	488	HIS
1	B	501	HIS
1	B	511	ASN
1	B	528	ASN
1	B	537	GLN
1	B	652	ASN
1	B	697	ASN
1	B	714	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 (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	380	2	26,33,33	1.51	6 (23%)	31,52,52	1.26	3 (9%)
3	ATP	B	880	2	26,33,33	1.65	5 (19%)	31,52,52	1.14	3 (9%)
4	LAR	A	901	-	30,31,31	1.55	7 (23%)	32,43,43	1.79	7 (21%)
4	LAR	B	921	-	30,31,31	1.60	4 (13%)	32,43,43	1.44	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	380	2	-	3/18/38/38	0/3/3/3
3	ATP	B	880	2	-	2/18/38/38	0/3/3/3
4	LAR	A	901	-	-	6/23/51/51	0/2/3/3
4	LAR	B	921	-	-	6/23/51/51	0/2/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	921	LAR	C20-N1	-5.60	1.26	1.34
3	B	880	ATP	C5'-C4'	4.43	1.65	1.51
4	A	901	LAR	C20-N1	-3.63	1.29	1.34
3	A	380	ATP	O2'-C2'	3.40	1.51	1.43
3	A	380	ATP	C5'-C4'	3.32	1.61	1.51
3	B	880	ATP	C2-N1	3.24	1.39	1.33
4	A	901	LAR	C19-C18	-3.09	1.47	1.53
3	B	880	ATP	C2'-C3'	-3.00	1.45	1.53
4	A	901	LAR	O2-C1	2.71	1.40	1.34
4	B	921	LAR	C19-C18	-2.57	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	LAR	O3-C13	2.52	1.50	1.44
3	A	380	ATP	C2-N1	2.47	1.38	1.33
4	B	921	LAR	C21-C3	2.46	1.57	1.50
3	B	880	ATP	C2'-C1'	-2.45	1.50	1.53
4	A	901	LAR	C18-N1	2.45	1.50	1.46
4	A	901	LAR	O1-C1	2.36	1.26	1.21
3	A	380	ATP	C2'-C1'	-2.24	1.50	1.53
4	B	921	LAR	O3-C13	2.18	1.49	1.44
3	A	380	ATP	C2-N3	2.15	1.35	1.32
3	A	380	ATP	C2'-C3'	-2.11	1.47	1.53
3	B	880	ATP	O2'-C2'	2.07	1.47	1.43
4	A	901	LAR	O4-C17	2.01	1.44	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	LAR	C19-S1-C20	5.95	95.19	92.00
4	B	921	LAR	C19-S1-C20	5.46	94.93	92.00
4	A	901	LAR	O5-C20-N1	3.89	131.05	126.81
3	A	380	ATP	C5-C6-N6	3.45	125.60	120.35
3	B	880	ATP	C1'-N9-C4	-3.25	120.93	126.64
3	A	380	ATP	C1'-N9-C4	-3.12	121.16	126.64
3	B	880	ATP	C5-C6-N6	2.98	124.89	120.35
4	B	921	LAR	C3-C2-C1	2.90	134.63	127.46
3	A	380	ATP	O3'-C3'-C4'	-2.88	102.73	111.05
4	A	901	LAR	C15-O2-C1	2.64	124.40	117.27
4	A	901	LAR	C3-C2-C1	2.52	133.71	127.46
4	B	921	LAR	O5-C20-N1	2.47	129.50	126.81
4	A	901	LAR	C21-C3-C4	2.29	119.12	115.27
4	A	901	LAR	O2-C15-C16	2.27	113.26	107.59
4	A	901	LAR	C21-C3-C2	-2.14	116.34	122.77
4	B	921	LAR	C21-C3-C2	-2.05	116.60	122.77
4	B	921	LAR	C21-C3-C4	2.05	118.71	115.27
3	B	880	ATP	O3'-C3'-C4'	-2.03	105.17	111.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	380	ATP	PB-O3B-PG-O3G
4	A	901	LAR	O3-C17-C18-C19
4	B	921	LAR	O3-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	B	880	ATP	PG-O3B-PB-O1B
4	B	921	LAR	C16-C15-O2-C1
4	A	901	LAR	O2-C1-C2-C3
4	A	901	LAR	C16-C15-O2-C1
4	B	921	LAR	O2-C1-C2-C3
3	A	380	ATP	PB-O3B-PG-O1G
3	A	380	ATP	PB-O3B-PG-O2G
4	A	901	LAR	C11-C10-C9-C8
3	B	880	ATP	PG-O3B-PB-O2B
4	B	921	LAR	C4-C5-C6-C7
4	A	901	LAR	C4-C5-C6-C7
4	B	921	LAR	C14-C15-O2-C1
4	A	901	LAR	C10-C11-C12-C13
4	B	921	LAR	O1-C1-C2-C3

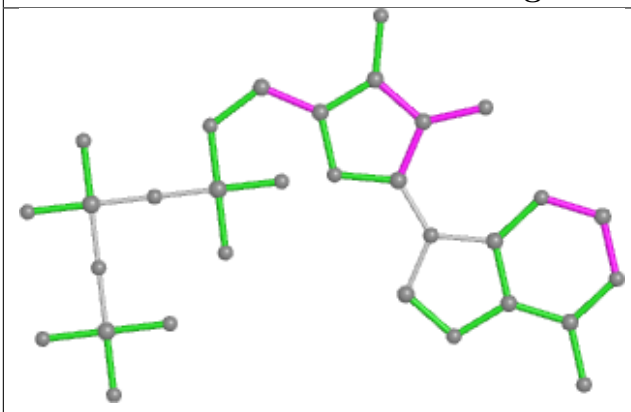
There are no ring outliers.

4 monomers are involved in 21 short contacts:

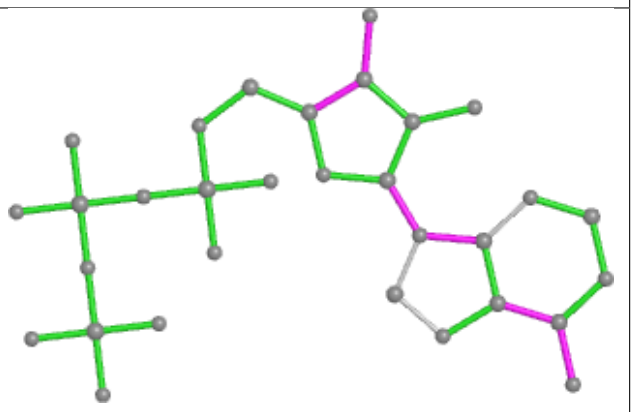
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	380	ATP	1	0
3	B	880	ATP	4	0
4	A	901	LAR	6	0
4	B	921	LAR	10	0

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.

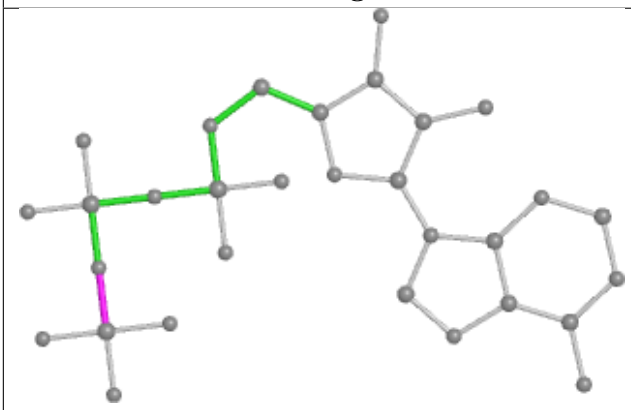
Ligand ATP A 380



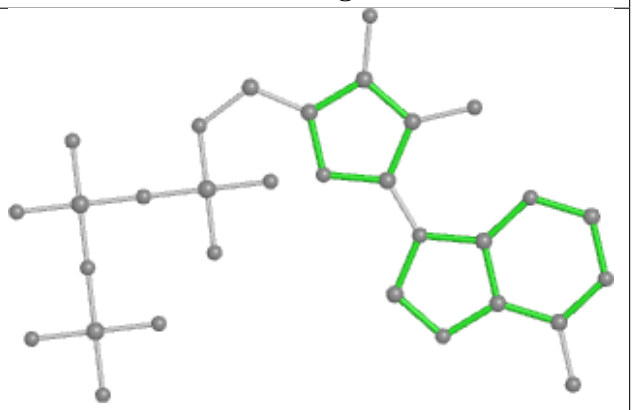
Bond lengths



Bond angles

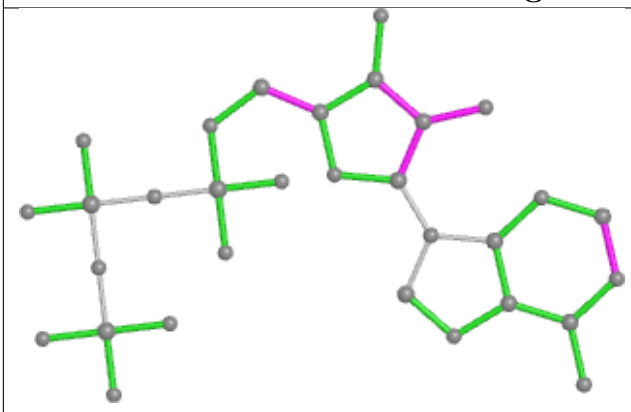


Torsions

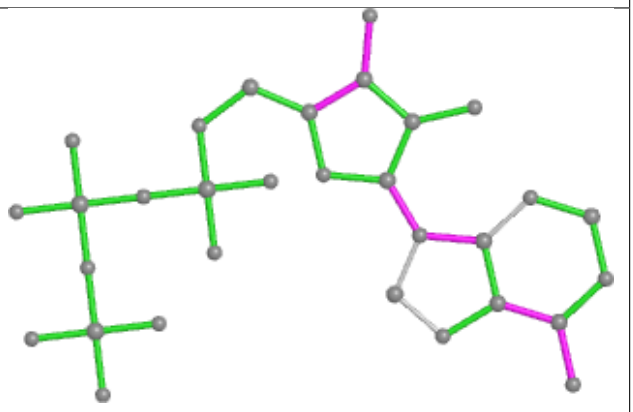


Rings

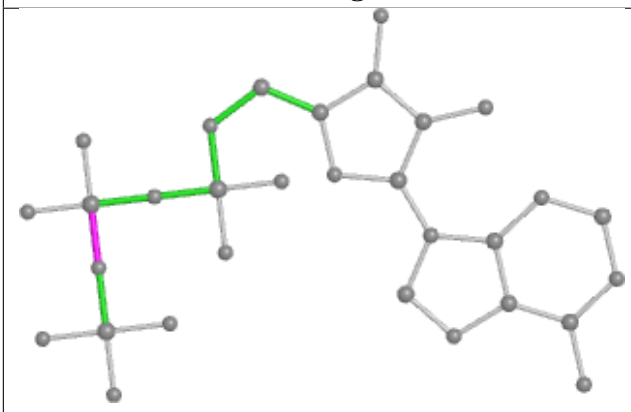
Ligand ATP B 880



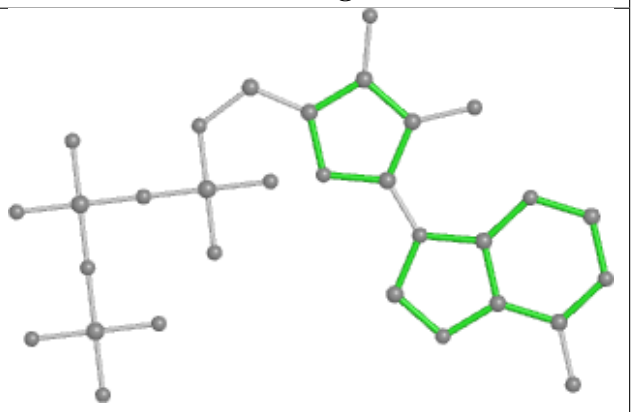
Bond lengths



Bond angles

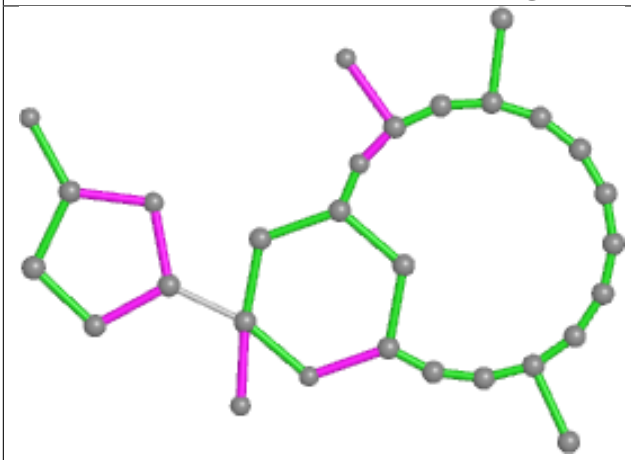


Torsions

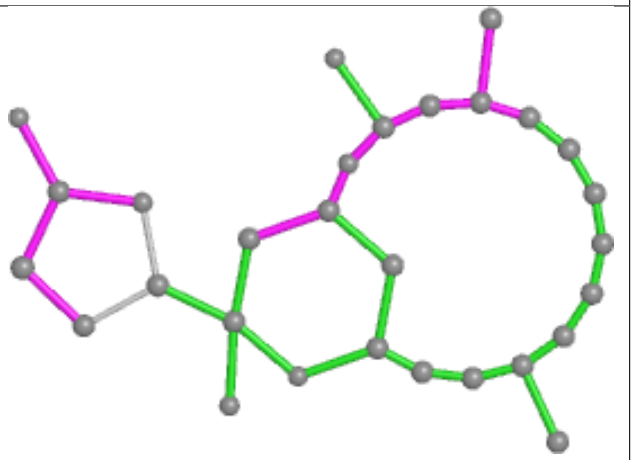


Rings

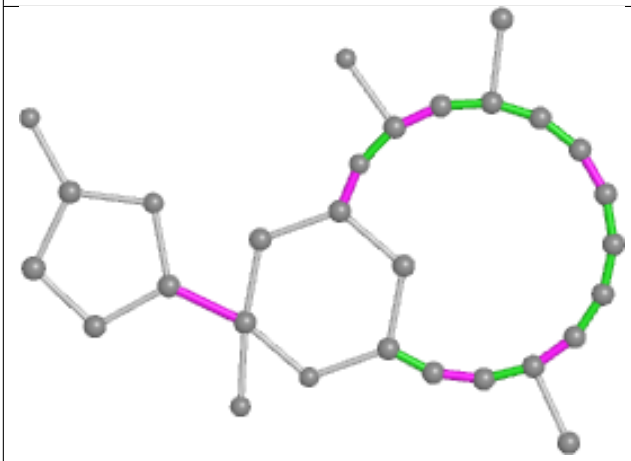
Ligand LAR A 901



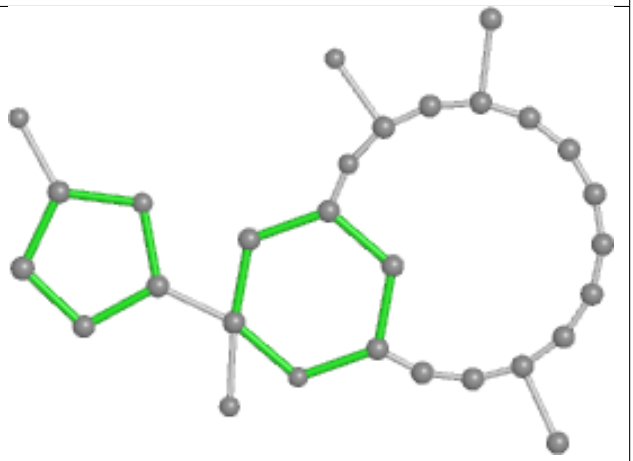
Bond lengths



Bond angles

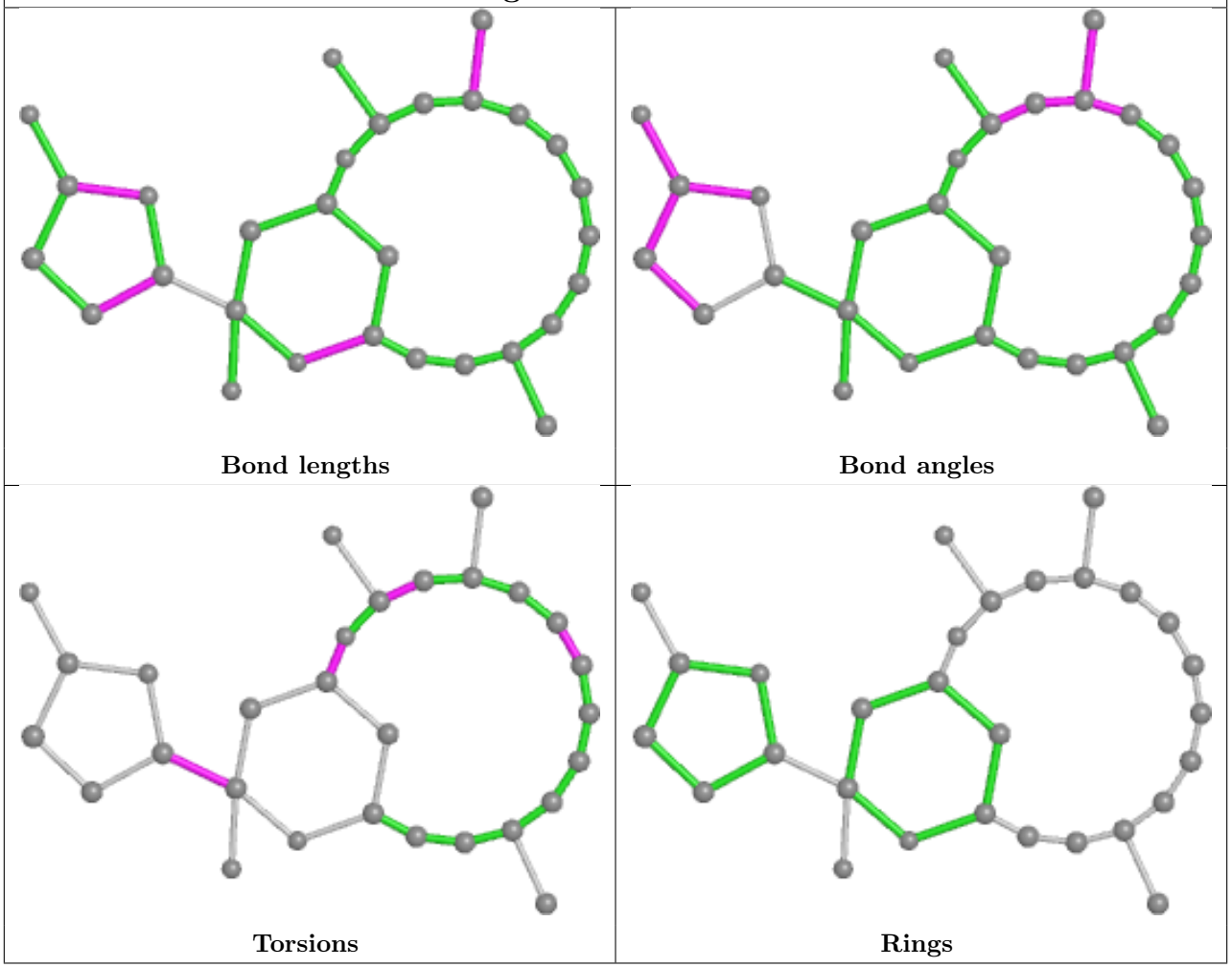


Torsions



Rings

Ligand LAR B 921



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.