Full wwPDB EM Validation Report

May 25, 2025 – 12:15 AM JST

PDB ID	:	9L4B / pdb_0000l4b
EMDB ID	:	EMD-62808
Title	:	Kinase domain of ATR bound with RP-3500
Authors	:	Wang, G.
Deposited on	:	2024-12-20
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

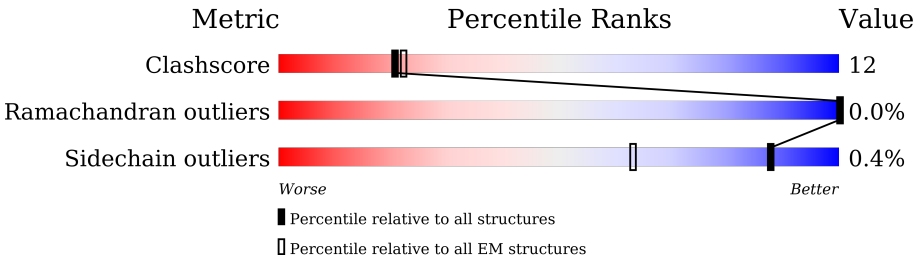
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2644	39% 11% 50%
1	B	2644	37% 13% 50%

2 Entry composition

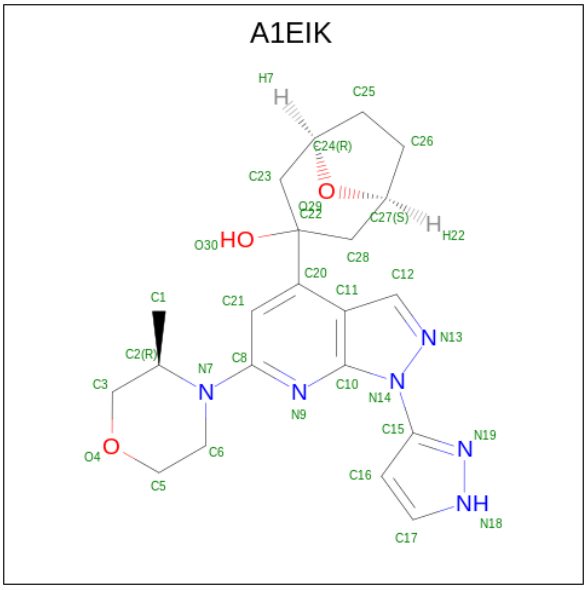
There are 3 unique types of molecules in this entry. The entry contains 40347 atoms, of which 19645 are hydrogens and 0 are deuteriums.

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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1335	Total	C	H	N	O	S	0	0
			19911	6499	9651	1785	1913	63		
1	B	1334	Total	C	H	N	O	S	0	0
			20372	6610	9994	1792	1907	69		

- Molecule 2 is RP-3500 (CCD ID: A1EIK) (formula: $C_{21}H_{26}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			30	21	6	3	
2	B	1	Total	C	N	O	0
			30	21	6	3	

- Molecule 3 is water.

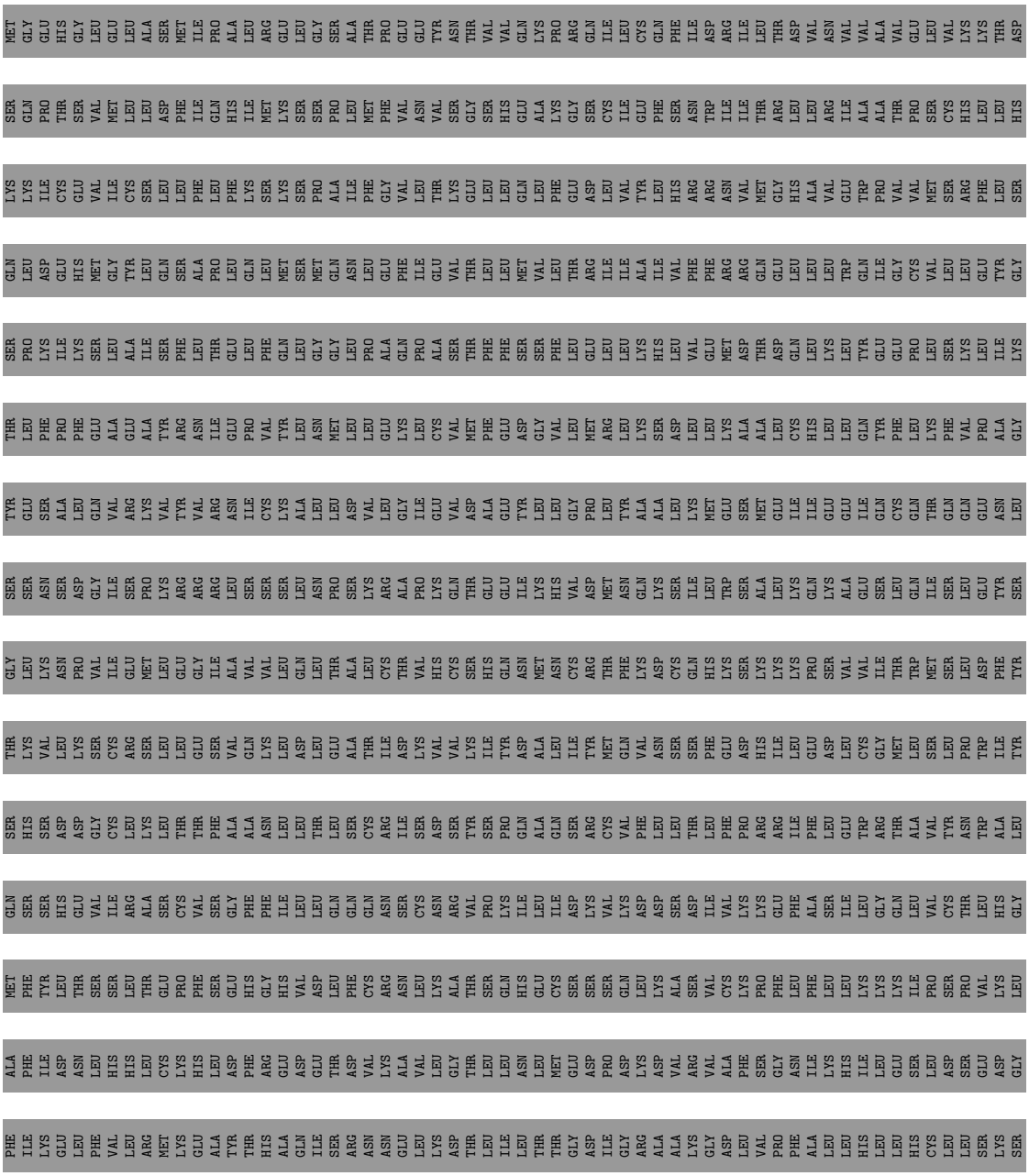
Mol	Chain	Residues	Atoms	AltConf
3	A	2	Total O 2 2	0
3	B	2	Total O 2 2	0

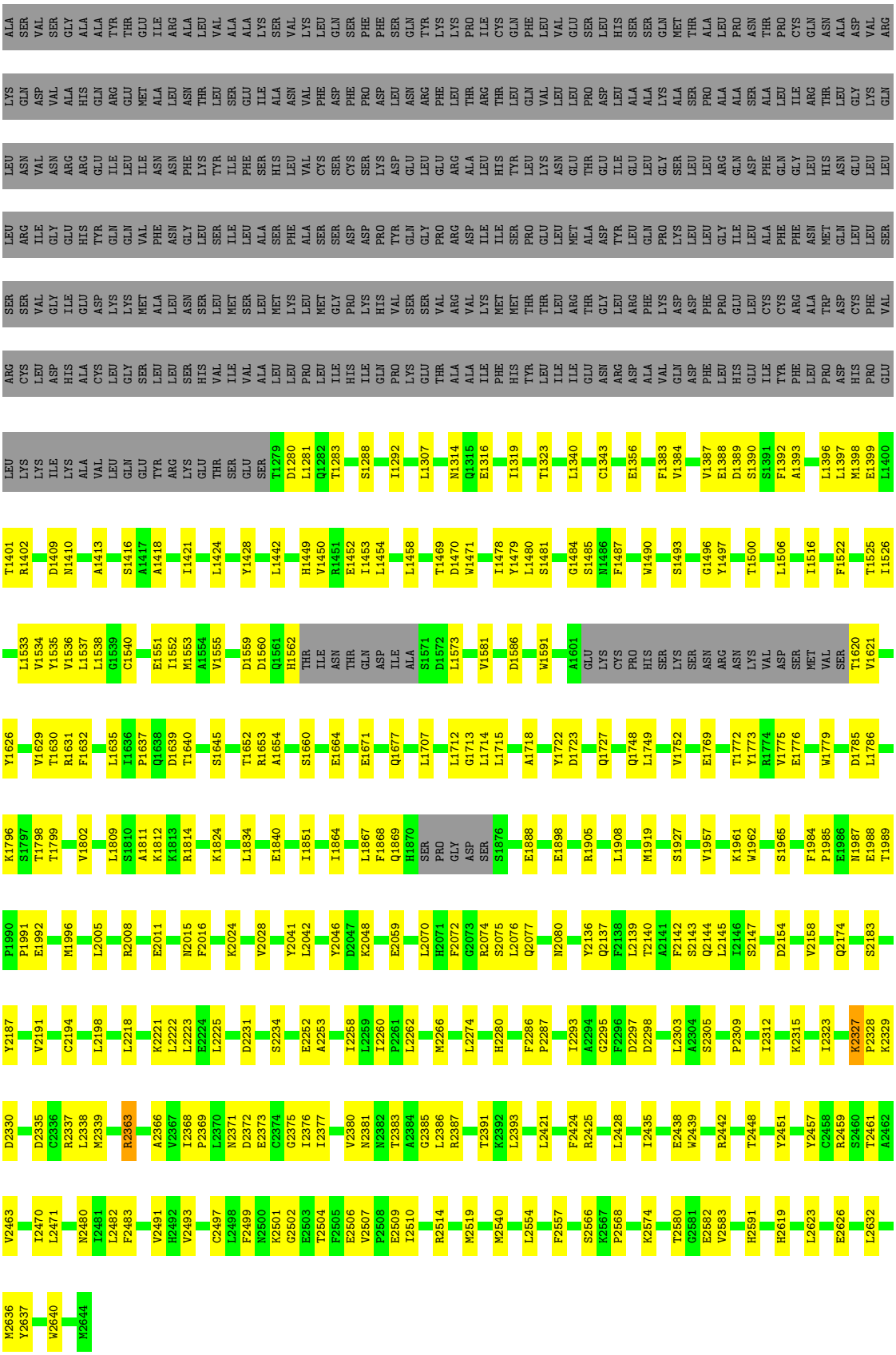
3 Residue-property plots (i)

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

- Molecule 1: Serine/threonine-protein kinase ATR

Chain A:

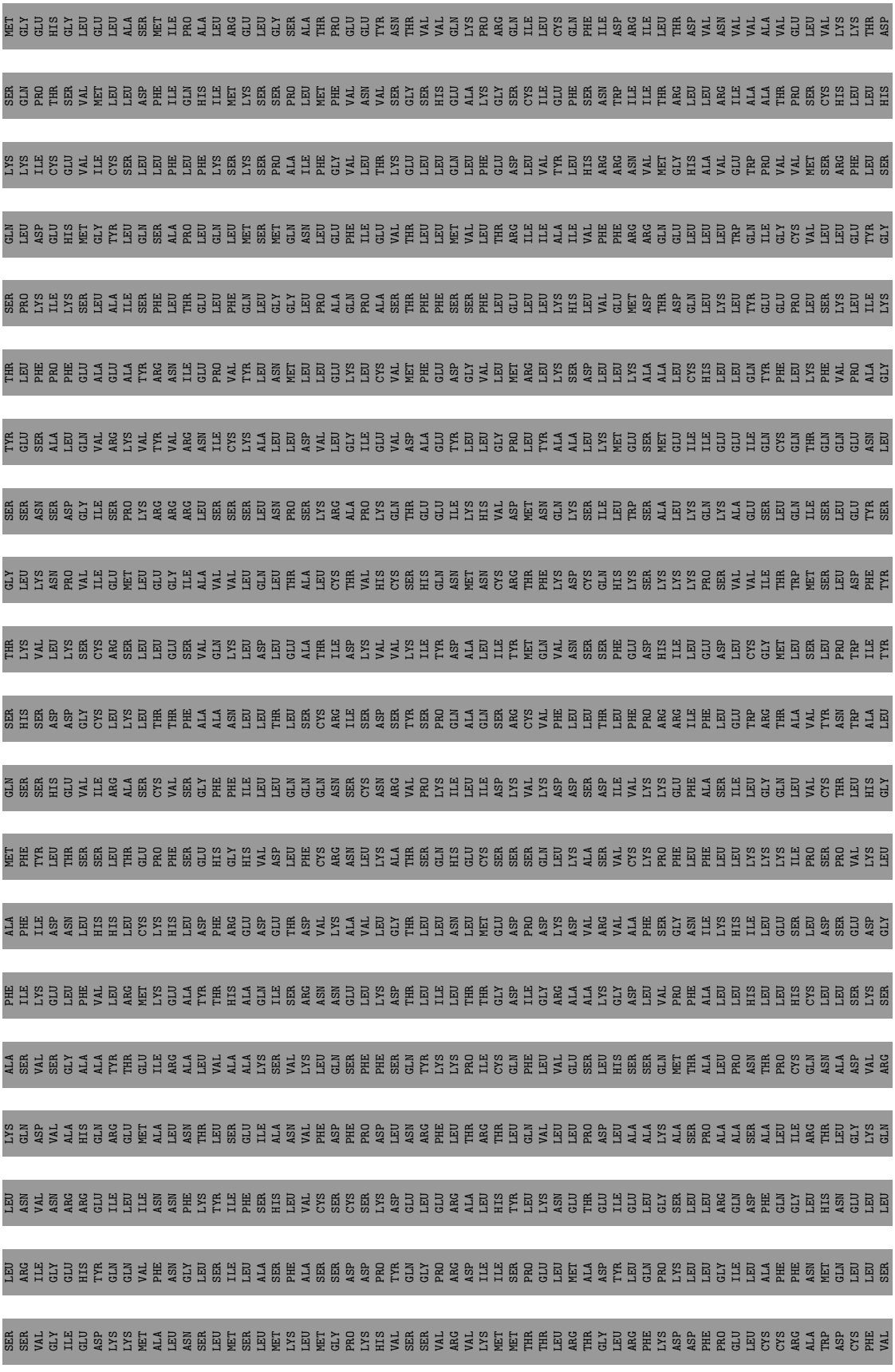


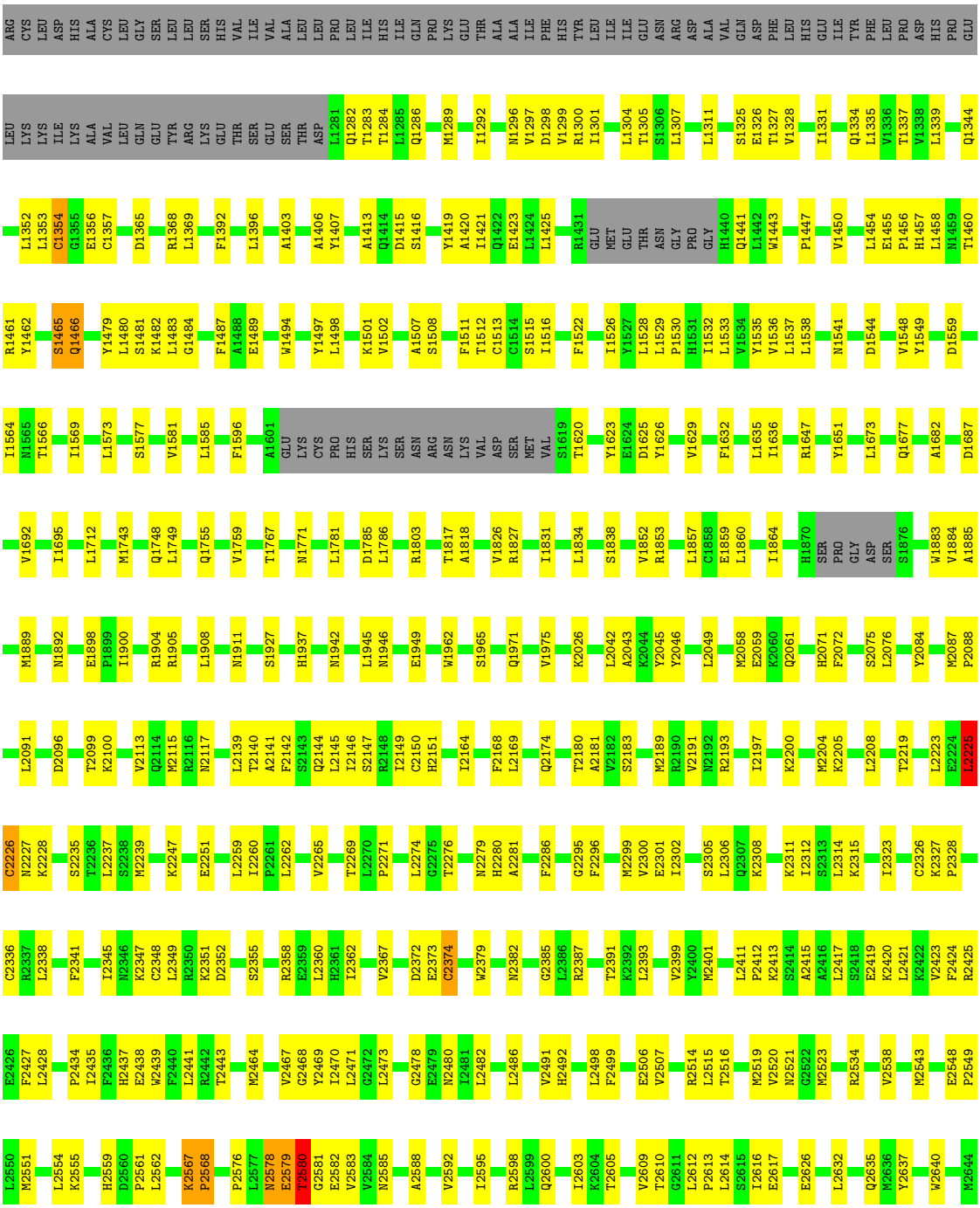


• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:


37%
13%
50%


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



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EIK

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	0.36	0/10488	0.42	0/14230
1	B	0.39	2/10604 (0.0%)	0.52	12/14369 (0.1%)
All	All	0.38	2/21092 (0.0%)	0.48	12/28599 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2225	LEU	C-O	-7.56	1.15	1.24
1	B	2373	GLU	C-O	-6.06	1.16	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2226	CYS	CB-CA-C	-13.30	88.25	110.85
1	B	2225	LEU	CA-C-O	-12.97	107.34	120.70
1	B	2326	CYS	N-CA-CB	9.85	125.70	109.94
1	B	2578	ASN	O-C-N	-9.71	109.68	122.59
1	B	2227	ASN	N-CA-C	-8.75	102.78	113.19
1	B	2372	ASP	N-CA-C	-7.88	102.38	110.97
1	B	2226	CYS	N-CA-CB	7.43	121.15	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2581	GLY	N-CA-C	-6.82	97.01	113.18
1	B	2372	ASP	O-C-N	6.21	128.49	122.03
1	B	2580	THR	N-CA-C	-5.19	99.74	110.80
1	B	2568	PRO	N-CA-C	-5.14	103.13	111.14
1	B	2579	GLU	N-CA-C	-5.09	106.58	112.89

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2363	ARG	Sidechain
1	B	1354	CYS	Peptide
1	B	1465	SER	Peptide
1	B	2225	LEU	Mainchain
1	B	2578	ASN	Mainchain
1	B	2580	THR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10260	9651	9686	200	0
1	B	10378	9994	10051	276	0
2	A	30	0	0	3	0
2	B	30	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	20702	19645	19737	476	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 12.

All (476) 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:2327:LYS:HZ2	2:A:2701:A1EIK:C16	1.71	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1304:LEU:HD22	1:B:1354:CYS:SG	2.05	0.96
1:A:1319:ILE:O	1:A:1323:THR:OG1	1.85	0.95
1:B:2276:THR:OG1	1:B:2279:ASN:OD1	1.88	0.91
1:B:2328:PRO:HA	1:B:2374:CYS:HB2	1.60	0.83
1:B:1466:GLN:OE1	1:B:1516:ILE:HB	1.80	0.82
1:A:2144:GLN:O	1:A:2147:SER:OG	1.96	0.82
1:A:1553:MET:HE1	1:A:1640:THR:HG21	1.59	0.82
1:B:2072:PHE:O	1:B:2075:SER:OG	2.00	0.80
1:A:1652:THR:HG21	1:A:2448:THR:HA	1.62	0.79
1:A:1307:LEU:O	1:A:1307:LEU:HD23	1.83	0.79
1:A:2568:PRO:O	1:A:2574:LYS:NZ	2.16	0.79
1:A:2457:TYR:OH	1:A:2519:MET:O	2.00	0.77
1:B:1344:GLN:NE2	1:B:1838:SER:OG	2.17	0.77
1:A:2080:ASN:ND2	1:A:2136:TYR:OH	2.18	0.76
1:A:1323:THR:HB	1:A:2274:LEU:HD11	1.67	0.76
1:B:2603:ILE:HG22	1:B:2605:THR:H	1.52	0.74
1:A:2327:LYS:NZ	2:A:2701:A1EIK:C16	2.49	0.74
1:B:1538:LEU:HD22	1:B:1625:ASP:HB3	1.70	0.74
1:B:1423:GLU:OE1	1:B:1423:GLU:N	2.21	0.73
1:B:2421:LEU:HD21	1:B:2425:ARG:HE	1.54	0.73
1:A:1393:ALA:HB1	1:A:1428:TYR:CZ	2.23	0.73
1:B:1307:LEU:O	1:B:1311:LEU:HG	1.87	0.72
1:B:2295:GLY:O	1:B:2315:LYS:N	2.21	0.72
1:B:1834:LEU:O	1:B:1838:SER:N	2.23	0.71
1:A:2385:GLY:HA2	1:A:2482:LEU:HD23	1.71	0.71
1:B:1327:THR:HG22	1:B:2269:THR:HG21	1.73	0.71
1:A:2252:GLU:OE1	1:A:2253:ALA:N	2.24	0.71
1:B:2259:LEU:HD21	1:B:2265:VAL:HG21	1.71	0.70
1:A:1553:MET:CE	1:A:1640:THR:HG21	2.21	0.69
1:A:2174:GLN:HA	1:A:2266:MET:HE1	1.72	0.69
1:B:2514:ARG:NH1	1:B:2640:TRP:O	2.25	0.69
1:B:2300:VAL:HG22	1:B:2312:ILE:HG22	1.75	0.68
1:A:2626:GLU:O	1:A:2632:LEU:HD12	1.94	0.68
1:B:1892:ASN:ND2	1:B:2352:ASP:OD2	2.27	0.68
1:A:2371:ASN:OD1	1:A:2372:ASP:N	2.26	0.67
1:A:2506:GLU:N	1:A:2506:GLU:OE1	2.27	0.67
1:B:2580:THR:HB	1:B:2582:GLU:HG3	1.77	0.67
1:B:2616:ILE:HG23	1:B:2617:GLU:H	1.60	0.67
1:B:2113:VAL:O	1:B:2117:ASN:ND2	2.29	0.66
1:B:2415:ALA:O	1:B:2420:LYS:NZ	2.28	0.66
1:B:1852:VAL:HG23	1:B:1900:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2580:THR:HG22	1:A:2582:GLU:H	1.60	0.66
1:B:1884:VAL:HG23	1:B:1885:ALA:H	1.61	0.66
1:A:2509:GLU:HA	1:A:2636:MET:HE1	1.78	0.66
1:A:2011:GLU:OE2	1:A:2048:LYS:NZ	2.24	0.65
1:B:2150:CYS:O	1:B:2580:THR:HG22	1.97	0.65
1:A:1905:ARG:HA	1:A:1908:LEU:HD12	1.78	0.65
1:B:1443:TRP:CZ3	1:B:1454:LEU:HD11	2.30	0.65
1:A:1323:THR:HB	1:A:2274:LEU:CD1	2.26	0.65
1:A:1888:GLU:CG	1:A:2274:LEU:HD22	2.27	0.65
1:A:1987:ASN:OD1	1:A:1988:GLU:N	2.29	0.64
1:B:2579:GLU:O	1:B:2580:THR:HG23	1.97	0.64
1:B:1673:LEU:HD22	1:B:1692:VAL:HG13	1.78	0.64
1:B:2411:LEU:HD11	1:B:2423:VAL:HG21	1.80	0.64
1:A:1671:GLU:OE1	1:A:1671:GLU:N	2.31	0.64
1:A:2072:PHE:O	1:A:2075:SER:OG	2.14	0.64
1:A:2143:SER:OG	1:A:2337:ARG:NH1	2.31	0.64
1:A:1398:MET:SD	1:A:1450:VAL:HG21	2.38	0.64
1:A:1586:ASP:OD2	1:A:1653:ARG:NH1	2.31	0.64
1:B:2164:ILE:HD11	1:B:2197:ILE:HD13	1.82	0.62
1:A:2225:LEU:HD23	1:A:2225:LEU:C	2.24	0.62
1:B:2247:LYS:NZ	1:B:2251:GLU:OE2	2.26	0.62
1:B:1573:LEU:O	1:B:1577:SER:OG	2.13	0.62
1:B:2341:PHE:CE2	1:B:2345:ILE:HD11	2.34	0.62
1:A:1496:GLY:O	1:A:1500:THR:HG23	2.00	0.62
1:A:1888:GLU:HG2	1:A:2274:LEU:HD22	1.80	0.62
1:A:2619:HIS:O	1:A:2623:LEU:HD23	2.00	0.62
1:B:1443:TRP:HZ3	1:B:1454:LEU:HD11	1.63	0.62
1:B:2362:ILE:HD11	1:B:2467:VAL:HG21	1.80	0.62
1:B:1898:GLU:OE1	1:B:1905:ARG:NH2	2.33	0.61
1:B:2144:GLN:O	1:B:2147:SER:OG	2.14	0.61
1:B:1420:ALA:HA	1:B:1513:CYS:SG	2.40	0.61
1:B:2045:TYR:CE2	1:B:2049:LEU:HD11	2.35	0.61
1:B:2499:PHE:CD1	1:B:2595:ILE:HD11	2.35	0.61
1:B:1884:VAL:HG23	1:B:1885:ALA:N	2.15	0.61
1:B:2146:ILE:O	1:B:2562:LEU:HD11	2.00	0.61
1:B:2411:LEU:HD13	1:B:2419:GLU:OE1	2.01	0.61
1:B:2189:MET:CE	1:B:2580:THR:HA	2.32	0.60
1:A:2323:ILE:HD13	1:A:2381:ASN:HD21	1.67	0.60
1:A:2380:VAL:HG23	1:A:2383:THR:HG21	1.83	0.60
1:A:1413:ALA:O	1:A:1416:SER:OG	2.19	0.60
1:B:1532:ILE:HA	1:B:1535:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2470:ILE:HD13	1:B:2543:MET:SD	2.42	0.59
1:B:2555:LYS:O	1:B:2559:HIS:ND1	2.35	0.59
1:B:1297:VAL:O	1:B:1300:ARG:N	2.35	0.59
1:B:2576:PRO:CB	1:B:2580:THR:C	2.75	0.59
1:A:2369:PRO:HA	1:A:2375:GLY:HA2	1.84	0.59
1:B:1304:LEU:HB2	1:B:1353:LEU:HD23	1.84	0.58
1:A:2386:LEU:HD13	1:A:2483:PHE:HE2	1.67	0.58
1:A:1723:ASP:OD2	1:A:1727:GLN:NE2	2.36	0.58
1:B:1532:ILE:O	1:B:1536:VAL:HG12	2.02	0.58
1:B:1537:LEU:HD11	1:B:1632:PHE:CB	2.33	0.58
1:B:1326:GLU:HB2	1:B:2351:LYS:HZ3	1.69	0.58
1:B:1785:ASP:OD1	1:B:1786:LEU:N	2.36	0.57
1:B:1529:LEU:HD23	1:B:1532:ILE:HD11	1.85	0.57
1:A:1775:VAL:HG11	1:A:1802:VAL:HG22	1.86	0.57
1:A:2077:GLN:O	1:A:2280:HIS:NE2	2.33	0.57
1:A:2258:ILE:O	1:A:2293:ILE:N	2.33	0.57
1:B:2026:LYS:NZ	1:B:2046:TYR:OH	2.20	0.57
1:B:2576:PRO:CB	1:B:2580:THR:O	2.53	0.57
1:B:1511:PHE:O	1:B:1515:SER:N	2.38	0.56
1:B:2200:LYS:HD2	1:B:2204:MET:HE3	1.86	0.56
1:B:2561:PRO:HB3	1:B:2582:GLU:HB3	1.86	0.56
1:A:1660:SER:O	1:A:1664:GLU:N	2.39	0.56
1:B:2387:ARG:O	1:B:2391:THR:HG23	2.06	0.56
1:A:1356:GLU:OE1	1:A:1824:LYS:NZ	2.37	0.56
1:B:2237:LEU:HD12	1:B:2302:ILE:HD11	1.88	0.56
1:B:1755:GLN:O	1:B:1759:VAL:HG23	2.06	0.56
1:B:2169:LEU:HD11	1:B:2204:MET:SD	2.46	0.56
1:B:2328:PRO:CA	1:B:2374:CYS:HB2	2.33	0.56
1:A:2637:TYR:HB3	1:A:2640:TRP:CZ3	2.41	0.56
1:B:1297:VAL:HG23	1:B:1298:ASP:N	2.21	0.56
1:A:1288:SER:O	1:A:1292:ILE:HG12	2.06	0.56
1:A:2154:ASP:O	1:A:2158:VAL:HG23	2.06	0.56
1:B:2417:LEU:HD13	1:B:2635:GLN:HE21	1.71	0.55
1:B:2189:MET:SD	1:B:2580:THR:HA	2.46	0.55
1:A:2554:LEU:O	1:A:2557:PHE:N	2.37	0.55
1:A:2393:LEU:HD11	1:A:2439:TRP:HB2	1.89	0.55
1:A:2514:ARG:NH1	1:A:2640:TRP:O	2.40	0.55
1:B:2411:LEU:HD11	1:B:2423:VAL:CG2	2.36	0.55
1:B:2626:GLU:O	1:B:2632:LEU:HD12	2.07	0.55
1:A:2386:LEU:HD13	1:A:2483:PHE:CE2	2.41	0.55
1:B:2585:ASN:HB3	1:B:2588:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2059:GLU:N	1:A:2059:GLU:OE1	2.40	0.54
1:B:2314:LEU:HD23	1:B:2314:LEU:H	1.72	0.54
1:A:1626:TYR:O	1:A:1630:THR:HG23	2.06	0.54
1:B:1942:ASN:HA	1:B:1945:LEU:HD12	1.88	0.54
1:A:1487:PHE:HA	1:A:1573:LEU:HD13	1.89	0.54
1:B:1549:TYR:CE1	1:B:1635:LEU:HG	2.42	0.54
1:B:1859:GLU:OE1	1:B:1904:ARG:NH2	2.35	0.54
1:B:1651:TYR:CZ	1:B:1682:ALA:HB1	2.43	0.54
1:B:1971:GLN:HE21	1:B:1975:VAL:HG23	1.72	0.54
1:B:2140:THR:O	1:B:2141:ALA:HB3	2.07	0.54
1:A:1772:THR:OG1	1:A:1799:THR:HG21	2.08	0.54
1:B:2183:SER:O	1:B:2191:VAL:HG13	2.07	0.54
1:A:1454:LEU:O	1:A:1458:LEU:N	2.41	0.54
1:B:2058:MET:O	1:B:2061:GLN:N	2.38	0.54
1:A:1387:VAL:HG23	1:A:1506:LEU:HD23	1.90	0.53
1:A:1416:SER:CB	1:A:1516:ILE:HD12	2.39	0.53
1:A:1639:ASP:OD1	1:A:1639:ASP:N	2.40	0.53
1:B:2237:LEU:N	1:B:2300:VAL:O	2.39	0.53
1:A:2218:LEU:O	1:A:2222:LEU:HD23	2.09	0.53
1:B:1883:TRP:O	1:B:1904:ARG:NH1	2.41	0.53
1:B:1479:TYR:C	1:B:1480:LEU:HD22	2.34	0.53
1:B:1898:GLU:OE2	1:B:1927:SER:OG	2.10	0.53
1:B:1529:LEU:HA	1:B:1532:ILE:HG12	1.90	0.53
1:B:2168:PHE:HD2	1:B:2208:LEU:HD21	1.74	0.53
1:B:2435:ILE:O	1:B:2438:GLU:N	2.42	0.53
1:A:1497:TYR:O	1:A:1500:THR:OG1	2.21	0.52
1:B:1392:PHE:CE2	1:B:1396:LEU:HD11	2.44	0.52
1:A:1785:ASP:OD1	1:A:1786:LEU:N	2.43	0.52
1:A:2497:CYS:SG	1:A:2502:GLY:N	2.83	0.52
1:B:1282:GLN:O	1:B:1286:GLN:NE2	2.42	0.52
1:B:1292:ILE:HG12	1:B:1304:LEU:HD23	1.90	0.52
1:A:1490:TRP:NE1	1:A:1551:GLU:OE2	2.40	0.52
1:A:1961:LYS:HE3	1:A:2005:LEU:HD11	1.91	0.52
1:B:2421:LEU:HD21	1:B:2425:ARG:NE	2.23	0.52
1:A:1392:PHE:CZ	1:A:1396:LEU:HD11	2.44	0.52
1:A:2393:LEU:CB	1:A:2435:ILE:HD12	2.40	0.52
1:B:1489:GLU:N	1:B:1489:GLU:OE1	2.42	0.52
1:B:2239:MET:HE2	1:B:2296:PHE:CB	2.40	0.52
1:B:2401:MET:HE3	1:B:2427:PHE:CE1	2.45	0.52
1:A:2042:LEU:HD11	1:A:2046:TYR:CE2	2.45	0.52
1:A:2421:LEU:HD21	1:A:2425:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2338:LEU:HD11	1:A:2471:LEU:HD13	1.92	0.51
1:B:2235:SER:O	1:B:2302:ILE:N	2.40	0.51
1:B:2299:MET:HE3	1:B:2301:GLU:HB3	1.92	0.51
1:A:2583:VAL:O	1:A:2583:VAL:HG23	2.10	0.51
1:A:1280:ASP:OD1	1:A:1283:THR:HG22	2.10	0.51
1:A:1864:ILE:O	1:A:1867:LEU:N	2.44	0.51
1:A:2501:LYS:O	1:A:2504:THR:OG1	2.20	0.51
1:B:2580:THR:HB	1:B:2582:GLU:CG	2.40	0.51
1:A:2510:ILE:HG22	1:A:2632:LEU:HD13	1.93	0.51
1:B:2280:HIS:O	1:B:2281:ALA:HB3	2.11	0.51
1:B:2382:ASN:HD22	1:B:2486:LEU:HD22	1.76	0.51
1:A:1409:ASP:OD1	1:A:1410:ASN:N	2.43	0.51
1:B:2338:LEU:C	1:B:2338:LEU:HD23	2.35	0.51
1:B:1577:SER:O	1:B:1581:VAL:HG12	2.11	0.51
1:B:2149:ILE:O	1:B:2193:ARG:NH1	2.44	0.51
1:A:2231:ASP:OD2	1:A:2234:SER:OG	2.20	0.51
1:A:2385:GLY:CA	1:A:2482:LEU:HD23	2.39	0.51
1:B:1502:VAL:CB	1:B:1535:TYR:CE2	2.94	0.51
1:A:2070:LEU:HD11	1:A:2074:ARG:HH21	1.76	0.51
1:A:2303:LEU:HD12	1:A:2309:PRO:HG2	1.93	0.50
1:A:2480:ASN:O	1:A:2493:VAL:HG22	2.11	0.50
1:A:1478:ILE:HG21	1:A:1493:SER:OG	2.11	0.50
1:B:2349:LEU:O	1:B:2355:SER:OG	2.24	0.50
1:B:2345:ILE:O	1:B:2348:CYS:N	2.43	0.50
1:A:1388:GLU:OE1	1:A:1535:TYR:OH	2.29	0.50
1:A:1645:SER:HB2	1:A:1654:ALA:HB2	1.92	0.50
1:B:1289:MET:HE1	1:B:1334:GLN:HB2	1.94	0.50
1:B:1497:TYR:O	1:B:1501:LYS:HG2	2.12	0.50
1:B:1508:SER:O	1:B:1512:THR:HG23	2.12	0.50
1:A:2297:ASP:OD1	1:A:2298:ASP:N	2.45	0.50
1:A:2393:LEU:HB2	1:A:2435:ILE:HD12	1.94	0.50
1:B:1300:ARG:O	1:B:1304:LEU:HG	2.12	0.50
1:B:1447:PRO:O	1:B:1450:VAL:N	2.44	0.50
1:B:1692:VAL:HA	1:B:1695:ILE:HG22	1.94	0.50
1:B:2189:MET:HE1	1:B:2580:THR:HA	1.92	0.50
1:B:2413:LYS:NZ	1:B:2506:GLU:O	2.41	0.50
1:B:2189:MET:CE	1:B:2580:THR:CA	2.90	0.50
1:B:2482:LEU:HB2	1:B:2491:VAL:HG13	1.94	0.49
1:A:1559:ASP:OD1	1:A:1559:ASP:N	2.41	0.49
1:B:1334:GLN:O	1:B:1337:THR:HG22	2.11	0.49
1:B:1403:ALA:O	1:B:1407:TYR:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1712:LEU:O	1:B:1712:LEU:HD23	2.13	0.49
1:B:2096:ASP:O	1:B:2099:THR:OG1	2.28	0.49
1:B:2259:LEU:HD21	1:B:2265:VAL:CG2	2.41	0.49
1:B:1305:THR:OG1	1:B:1353:LEU:HD21	2.13	0.49
1:B:2084:TYR:OH	1:B:2347:LYS:NZ	2.27	0.49
1:A:1809:LEU:O	1:A:1812:LYS:N	2.46	0.49
1:A:1888:GLU:HG3	1:A:2274:LEU:HD22	1.93	0.49
1:B:2180:THR:O	1:B:2183:SER:OG	2.17	0.49
1:B:1949:GLU:OE1	1:B:1949:GLU:N	2.46	0.49
1:A:1919:MET:N	1:A:1919:MET:HE2	2.27	0.49
1:A:2024:LYS:O	1:A:2028:VAL:HG23	2.13	0.49
1:B:2580:THR:HB	1:B:2582:GLU:H	1.78	0.49
1:A:1652:THR:HG23	1:A:2451:TYR:HB2	1.93	0.49
1:A:2424:PHE:HA	1:A:2428:LEU:HD12	1.95	0.49
1:B:2043:ALA:HB2	1:B:2071:HIS:HB2	1.94	0.49
1:B:2616:ILE:HG23	1:B:2617:GLU:N	2.26	0.49
1:B:1860:LEU:HD12	1:B:1864:ILE:HG12	1.96	0.48
1:B:2393:LEU:HD11	1:B:2439:TRP:HB2	1.95	0.48
1:A:1340:LEU:O	1:A:1343:CYS:N	2.46	0.48
1:A:1637:PRO:O	1:A:1640:THR:OG1	2.26	0.48
1:B:1532:ILE:HA	1:B:1535:TYR:CE1	2.48	0.48
1:B:2087:MET:SD	1:B:2091:LEU:HD11	2.54	0.48
1:A:1840:GLU:OE2	1:A:1840:GLU:N	2.46	0.48
1:A:1962:TRP:O	1:A:1965:SER:OG	2.28	0.48
1:B:1481:SER:C	1:B:1483:LEU:H	2.22	0.48
1:A:1898:GLU:OE2	1:A:1927:SER:OG	2.27	0.48
1:B:1365:ASP:N	1:B:1889:MET:O	2.43	0.48
1:A:2435:ILE:O	1:A:2438:GLU:N	2.42	0.48
1:B:1465:SER:O	1:B:1466:GLN:NE2	2.47	0.48
1:B:1803:ARG:HB3	1:B:1826:VAL:CG1	2.44	0.48
1:B:1296:ASN:HD22	1:B:1299:VAL:HG23	1.79	0.48
1:B:1564:ILE:HG23	1:B:1564:ILE:O	2.13	0.48
1:B:2169:LEU:HD22	1:B:2205:LYS:HD3	1.96	0.48
1:A:1470:ASP:OD1	1:A:1471:TRP:N	2.47	0.47
1:A:2194:CYS:O	1:A:2198:LEU:HD13	2.14	0.47
1:A:2366:ALA:HB1	1:A:2368:ILE:HD11	1.95	0.47
1:A:2328:PRO:O	1:A:2329:LYS:C	2.57	0.47
1:A:2376:ILE:HG13	1:A:2376:ILE:O	2.14	0.47
1:B:1962:TRP:O	1:B:1965:SER:OG	2.29	0.47
1:B:1817:THR:HG23	1:B:1818:ALA:N	2.27	0.47
1:B:1421:ILE:HG21	1:B:1457:HIS:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:LEU:O	1:A:1752:VAL:HB	2.14	0.47
1:A:2459:ARG:O	1:A:2463:VAL:HG23	2.15	0.47
1:B:2174:GLN:N	1:B:2174:GLN:OE1	2.48	0.47
1:B:1415:ASP:O	1:B:1419:TYR:N	2.47	0.47
1:B:1620:THR:HG23	1:B:1623:TYR:H	1.79	0.47
1:B:1327:THR:CG2	1:B:2269:THR:HG21	2.43	0.46
1:B:1416:SER:OG	1:B:1466:GLN:NE2	2.48	0.46
1:B:1511:PHE:CE2	1:B:1535:TYR:CE1	3.03	0.46
1:B:1549:TYR:CZ	1:B:1635:LEU:HG	2.50	0.46
1:B:2059:GLU:OE1	1:B:2059:GLU:N	2.40	0.46
1:A:2015:ASN:OD1	1:A:2016:PHE:N	2.48	0.46
1:B:2260:ILE:O	1:B:2262:LEU:N	2.45	0.46
1:B:2580:THR:HB	1:B:2582:GLU:CB	2.45	0.46
1:A:1677:GLN:HG2	1:A:1707:LEU:HD23	1.97	0.46
1:A:1984:PHE:N	1:A:1985:PRO:HD3	2.30	0.46
1:A:2262:LEU:O	1:A:2266:MET:HG2	2.15	0.46
1:A:2499:PHE:O	1:A:2591:HIS:CE1	2.68	0.46
1:B:1335:LEU:O	1:B:1339:LEU:HG	2.15	0.46
1:B:1458:LEU:C	1:B:1460:THR:H	2.22	0.46
1:B:1297:VAL:O	1:B:1301:ILE:HD12	2.15	0.46
1:B:2189:MET:HE1	1:B:2580:THR:CA	2.46	0.46
1:B:1677:GLN:HG3	1:B:1692:VAL:HG11	1.98	0.46
1:B:2614:LEU:N	1:B:2614:LEU:HD12	2.31	0.46
1:A:1393:ALA:HB1	1:A:1428:TYR:OH	2.16	0.46
1:B:1441:GLN:OE1	1:B:1441:GLN:N	2.40	0.46
1:A:1536:VAL:O	1:A:1540:CYS:N	2.48	0.46
1:A:2470:ILE:HD11	1:A:2540:MET:HE1	1.98	0.46
1:A:2183:SER:O	1:A:2191:VAL:HG22	2.17	0.46
1:A:2491:VAL:HG13	1:A:2491:VAL:O	2.16	0.46
1:B:2609:VAL:HG23	1:B:2609:VAL:O	2.15	0.45
1:B:1283:THR:HG23	1:B:1284:THR:N	2.31	0.45
1:A:1525:THR:O	1:A:1526:ILE:C	2.59	0.45
1:A:2260:ILE:O	1:A:2262:LEU:N	2.48	0.45
1:B:2180:THR:OG1	1:B:2219:THR:HG21	2.16	0.45
1:A:1769:GLU:N	1:A:1769:GLU:OE1	2.48	0.45
1:A:2295:GLY:O	1:A:2315:LYS:N	2.37	0.45
1:A:1469:THR:HG22	1:A:1471:TRP:N	2.31	0.45
1:A:1776:GLU:HA	1:A:1779:TRP:CD1	2.51	0.45
1:A:2174:GLN:CA	1:A:2266:MET:HE1	2.43	0.45
1:B:1307:LEU:HD11	1:B:1311:LEU:HD21	1.98	0.45
1:A:1957:VAL:HG13	1:A:2005:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2439:TRP:CE2	1:B:2443:THR:HG21	2.52	0.45
1:A:1416:SER:HA	1:A:1516:ILE:HD12	1.99	0.45
1:A:2330:ASP:N	1:A:2373:GLU:O	2.46	0.45
1:B:1328:VAL:HG21	1:B:1369:LEU:HD23	1.99	0.45
1:A:1469:THR:HG22	1:A:1471:TRP:H	1.82	0.45
1:B:1538:LEU:HD22	1:B:1625:ASP:CB	2.44	0.45
1:B:2151:HIS:O	1:B:2193:ARG:NH2	2.48	0.45
1:A:1418:ALA:O	1:A:1421:ILE:HG22	2.17	0.45
1:B:1537:LEU:HD11	1:B:1632:PHE:HB3	1.99	0.45
1:B:1827:ARG:O	1:B:1831:ILE:HD12	2.17	0.45
1:A:1383:PHE:O	1:A:1384:VAL:C	2.60	0.45
1:A:1560:ASP:O	1:A:1562:HIS:ND1	2.49	0.45
1:A:1718:ALA:O	1:A:1722:TYR:CD2	2.70	0.45
1:A:2421:LEU:HD21	1:A:2425:ARG:HH12	1.82	0.45
1:B:2515:LEU:HD11	1:B:2523:MET:HE1	1.99	0.45
1:B:2567:LYS:HB2	1:B:2568:PRO:HD2	1.98	0.45
1:B:1325:SER:HA	1:B:2271:PRO:HA	1.99	0.44
1:B:1392:PHE:CZ	1:B:1396:LEU:HD11	2.52	0.44
1:B:2583:VAL:HG23	1:B:2583:VAL:O	2.16	0.44
1:A:1316:GLU:OE1	1:A:1316:GLU:N	2.37	0.44
1:B:1484:GLY:O	1:B:1573:LEU:HD12	2.18	0.44
1:B:1581:VAL:O	1:B:1585:LEU:HD13	2.16	0.44
1:B:2100:LYS:HG3	1:B:2115:MET:HE1	1.99	0.44
1:B:2140:THR:O	1:B:2141:ALA:CB	2.65	0.44
1:B:2139:LEU:HD21	1:B:2286:PHE:CZ	2.52	0.44
1:B:2385:GLY:HA2	1:B:2482:LEU:HD23	1.99	0.44
1:B:2600:GLN:O	1:B:2614:LEU:HD23	2.16	0.44
1:A:2223:LEU:C	1:A:2223:LEU:HD12	2.42	0.44
1:A:2507:VAL:HG11	1:A:2637:TYR:H	1.81	0.44
1:A:2566:SER:O	1:A:2566:SER:OG	2.32	0.44
1:B:1421:ILE:HD11	1:B:1425:LEU:HD13	2.00	0.44
1:B:2534:ARG:O	1:B:2538:VAL:HG23	2.17	0.44
1:A:1533:LEU:O	1:A:1537:LEU:HD13	2.16	0.44
1:B:1331:ILE:HD12	1:B:1331:ILE:H	1.83	0.44
1:B:1566:THR:O	1:B:1569:ILE:HG22	2.18	0.44
1:A:1449:HIS:O	1:A:1452:GLU:HG3	2.18	0.44
1:B:1297:VAL:HG23	1:B:1298:ASP:H	1.83	0.44
1:B:1651:TYR:CE2	1:B:1682:ALA:HB1	2.53	0.44
1:B:2399:VAL:O	1:B:2399:VAL:HG13	2.18	0.44
1:B:2076:LEU:HD13	1:B:2087:MET:HE2	1.98	0.44
1:B:2226:CYS:C	1:B:2228:LYS:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:ARG:O	1:A:1635:LEU:HD23	2.18	0.44
1:A:2482:LEU:HB2	1:A:2491:VAL:HG13	2.00	0.44
1:A:1712:LEU:HB3	1:A:1714:LEU:HD23	1.98	0.44
1:A:1989:THR:O	1:A:1991:PRO:HD3	2.18	0.43
1:A:2076:LEU:O	1:A:2137:GLN:NE2	2.51	0.43
1:A:1418:ALA:HA	1:A:1421:ILE:HG22	2.00	0.43
1:B:2424:PHE:HA	1:B:2428:LEU:HD12	1.99	0.43
1:A:1591:TRP:CE3	1:A:1629:VAL:HG11	2.53	0.43
1:B:1356:GLU:O	1:B:1357:CYS:C	2.60	0.43
1:B:1454:LEU:C	1:B:1454:LEU:HD12	2.43	0.43
1:B:2239:MET:HE2	1:B:2296:PHE:HB3	2.01	0.43
1:A:1552:ILE:HG23	1:A:1581:VAL:HG21	2.00	0.43
1:A:2008:ARG:NH2	1:A:2041:TYR:OH	2.51	0.43
1:B:1942:ASN:O	1:B:1946:ASN:ND2	2.51	0.43
1:A:1397:LEU:HD22	1:A:1424:LEU:HD13	1.99	0.43
1:A:2507:VAL:HG11	1:A:2637:TYR:N	2.34	0.43
1:B:1413:ALA:O	1:B:1416:SER:HB2	2.19	0.43
1:B:2302:ILE:HG22	1:B:2308:LYS:HE2	1.99	0.43
1:A:1484:GLY:HA2	1:A:1490:TRP:HB2	2.01	0.43
1:B:2379:TRP:HA	2:B:2701:A1EIK:C3	2.48	0.43
1:B:2411:LEU:HB3	1:B:2412:PRO:HD2	2.01	0.43
1:B:2612:LEU:N	1:B:2613:PRO:HD3	2.34	0.43
1:A:2187:TYR:CZ	1:A:2574:LYS:HA	2.53	0.43
1:B:2142:PHE:HA	1:B:2145:LEU:HD12	2.00	0.43
1:B:2554:LEU:HD21	1:B:2595:ILE:HD13	2.00	0.43
1:B:1687:ASP:OD2	1:B:2358:ARG:NH1	2.51	0.43
1:B:2516:THR:O	1:B:2520:VAL:HG23	2.18	0.43
1:B:2580:THR:HB	1:B:2582:GLU:HB2	2.01	0.43
1:A:1811:ALA:O	1:A:1814:ARG:HD2	2.19	0.43
1:A:1868:PHE:O	1:A:1869:GLN:C	2.61	0.43
1:B:1626:TYR:HA	1:B:1629:VAL:HG22	2.00	0.43
1:B:2168:PHE:CD2	1:B:2208:LEU:HD21	2.54	0.43
1:B:2507:VAL:HG11	1:B:2637:TYR:N	2.34	0.43
1:B:1743:MET:O	1:B:1748:GLN:HB2	2.19	0.43
1:B:1767:THR:O	1:B:1771:ASN:N	2.52	0.43
1:B:2328:PRO:O	1:B:2374:CYS:CB	2.67	0.43
1:B:2338:LEU:HD13	1:B:2498:LEU:HD11	2.01	0.43
1:A:1522:PHE:O	1:A:1526:ILE:HG12	2.18	0.42
1:A:2393:LEU:HD22	1:A:2442:ARG:HH11	1.84	0.42
1:B:1352:LEU:HA	1:B:1831:ILE:HD13	2.00	0.42
1:B:2341:PHE:CE2	1:B:2471:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2464:MET:HG2	1:B:2492:HIS:CD2	2.54	0.42
1:A:2457:TYR:O	1:A:2461:THR:HG22	2.18	0.42
1:B:2468:GLY:O	1:B:2473:LEU:N	2.43	0.42
1:B:2610:THR:O	1:B:2610:THR:HG22	2.19	0.42
1:A:2335:ASP:O	1:A:2339:MET:HG2	2.20	0.42
1:B:1461:ARG:O	1:B:1462:TYR:C	2.61	0.42
1:B:1892:ASN:HB2	1:B:2352:ASP:HA	2.01	0.42
1:B:2180:THR:HG23	1:B:2181:ALA:N	2.33	0.42
1:B:2434:PRO:HB2	1:B:2521:ASN:ND2	2.34	0.42
1:B:2437:HIS:O	1:B:2441:LEU:HG	2.20	0.42
1:A:1796:LYS:O	1:A:1798:THR:HG23	2.19	0.42
1:A:2323:ILE:N	1:A:2323:ILE:HD12	2.35	0.42
1:B:1511:PHE:CD1	1:B:1528:LEU:HD22	2.55	0.42
1:B:1596:PHE:HB2	1:B:1626:TYR:CZ	2.55	0.42
1:B:1632:PHE:O	1:B:1635:LEU:N	2.52	0.42
1:A:1387:VAL:HA	1:A:1392:PHE:CE2	2.55	0.42
1:B:1507:ALA:O	1:B:1511:PHE:CD2	2.73	0.42
1:B:2311:LYS:HE2	1:B:2323:ILE:HG21	2.02	0.42
1:B:1403:ALA:O	1:B:1406:ALA:N	2.49	0.42
1:B:1559:ASP:OD1	1:B:1647:ARG:NH1	2.38	0.42
1:B:2274:LEU:O	1:B:2274:LEU:HG	2.20	0.42
1:A:2136:TYR:HH	1:A:2280:HIS:CB	2.33	0.42
1:B:1537:LEU:HD11	1:B:1632:PHE:CG	2.55	0.42
1:B:1908:LEU:O	1:B:1911:ASN:O	2.38	0.42
1:B:2087:MET:HB3	1:B:2088:PRO:HD3	2.00	0.42
1:B:2139:LEU:O	1:B:2142:PHE:HB2	2.20	0.42
1:B:2548:GLU:HB2	1:B:2549:PRO:HD3	2.02	0.42
1:B:1487:PHE:N	1:B:1573:LEU:HD11	2.35	0.42
1:B:1502:VAL:CB	1:B:1536:VAL:HA	2.50	0.42
1:B:1522:PHE:O	1:B:1526:ILE:HG12	2.20	0.42
1:A:1534:VAL:O	1:A:1538:LEU:HG	2.19	0.42
1:A:2368:ILE:O	1:A:2376:ILE:N	2.40	0.42
1:B:1569:ILE:HD12	1:B:1569:ILE:HA	1.93	0.42
1:B:2336:CYS:HA	1:B:2367:VAL:HG13	2.02	0.42
1:B:2401:MET:HE3	1:B:2427:PHE:HE1	1.84	0.42
1:A:1281:LEU:HD13	1:A:1314:ASN:CG	2.45	0.41
1:B:1328:VAL:HG13	1:B:1368:ARG:HB3	2.01	0.41
1:B:1481:SER:O	1:B:1482:LYS:HB2	2.20	0.41
1:B:2189:MET:HE1	1:B:2579:GLU:C	2.44	0.41
1:A:1748:GLN:O	1:A:1752:VAL:HG23	2.20	0.41
1:A:2139:LEU:HD21	1:A:2286:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1296:ASN:ND2	1:B:1299:VAL:HG23	2.35	0.41
1:B:1356:GLU:CG	1:B:1827:ARG:HD3	2.50	0.41
1:B:2580:THR:CB	1:B:2582:GLU:HB2	2.50	0.41
1:A:2510:ILE:HG21	1:A:2632:LEU:HD22	2.02	0.41
1:B:1884:VAL:CG2	1:B:1885:ALA:H	2.32	0.41
1:B:2226:CYS:C	1:B:2228:LYS:H	2.28	0.41
1:B:2421:LEU:C	1:B:2421:LEU:HD23	2.45	0.41
1:B:2469:TYR:O	1:B:2598:ARG:NE	2.54	0.41
1:B:2499:PHE:CE1	1:B:2595:ILE:HD11	2.55	0.41
1:A:2221:LYS:N	1:A:2221:LYS:HD2	2.35	0.41
1:B:1532:ILE:HG13	1:B:1533:LEU:N	2.35	0.41
1:A:1390:SER:O	1:A:1442:LEU:HD21	2.20	0.41
1:A:1620:THR:OG1	1:A:1621:VAL:N	2.53	0.41
1:A:1772:THR:HG23	1:A:1773:TYR:N	2.36	0.41
1:A:2387:ARG:O	1:A:2391:THR:HG23	2.21	0.41
1:B:1421:ILE:HG21	1:B:1457:HIS:HB2	2.03	0.41
1:B:1529:LEU:N	1:B:1530:PRO:HD2	2.36	0.41
1:B:2514:ARG:HG2	1:B:2519:MET:SD	2.60	0.41
1:B:2223:LEU:O	1:B:2223:LEU:HD23	2.21	0.41
1:A:1280:ASP:O	1:A:1281:LEU:HB3	2.20	0.41
1:A:1713:GLY:O	1:A:1715:LEU:HD22	2.21	0.41
1:B:2387:ARG:HG3	1:B:2478:GLY:HA3	2.02	0.41
1:A:1288:SER:OG	1:A:1307:LEU:HD12	2.21	0.41
1:A:1389:ASP:OD1	1:A:1390:SER:N	2.54	0.41
1:A:1399:GLU:OE2	1:A:1402:ARG:NH2	2.50	0.41
1:A:1428:TYR:CE2	1:A:1442:LEU:HD13	2.56	0.41
1:A:1479:TYR:CD2	1:A:1480:LEU:HG	2.55	0.41
1:A:1537:LEU:HD21	1:A:1632:PHE:CG	2.56	0.41
1:A:1551:GLU:O	1:A:1555:VAL:HG23	2.21	0.41
1:A:1591:TRP:CZ3	1:A:1629:VAL:HG11	2.56	0.41
1:A:2137:GLN:O	1:A:2140:THR:HG22	2.21	0.41
1:A:2174:GLN:NE2	1:A:2286:PHE:CD2	2.89	0.41
1:B:1421:ILE:HD11	1:B:1454:LEU:HD13	2.03	0.41
1:B:1494:TRP:CE2	1:B:1498:LEU:HD11	2.56	0.41
1:B:1632:PHE:O	1:B:1636:ILE:HD12	2.21	0.41
1:A:1772:THR:CB	1:A:1799:THR:HG21	2.51	0.41
1:B:1339:LEU:CD2	1:B:1354:CYS:SG	3.09	0.41
1:B:1498:LEU:CD2	1:B:1548:VAL:HG22	2.51	0.41
1:A:1560:ASP:O	1:A:1562:HIS:CE1	2.74	0.40
1:A:1834:LEU:HD21	1:A:1851:ILE:HG13	2.03	0.40
1:A:1992:GLU:O	1:A:1996:MET:N	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2225:LEU:HD11	1:A:2312:ILE:HG21	2.03	0.40
1:A:2377:ILE:HG21	2:A:2701:A1EIK:C6	2.51	0.40
1:B:1884:VAL:CG2	1:B:1885:ALA:N	2.83	0.40
1:B:1937:HIS:HB3	1:B:1962:TRP:HE1	1.85	0.40
1:A:2221:LYS:HE3	1:A:2221:LYS:HA	2.03	0.40
1:A:2574:LYS:H	1:A:2574:LYS:HD2	1.85	0.40
1:B:1455:GLU:N	1:B:1456:PRO:HD2	2.36	0.40
1:B:1479:TYR:O	1:B:1480:LEU:HD22	2.21	0.40
1:B:1749:LEU:HD23	1:B:1781:LEU:HG	2.02	0.40
1:B:2305:SER:O	1:B:2306:LEU:C	2.64	0.40
1:A:1401:THR:HG21	1:A:1450:VAL:HA	2.03	0.40
1:B:2042:LEU:HD23	1:B:2071:HIS:CD2	2.56	0.40
1:B:2515:LEU:HD12	1:B:2515:LEU:HA	1.86	0.40
1:A:1449:HIS:O	1:A:1453:ILE:HG12	2.22	0.40
1:A:1481:SER:O	1:A:1485:SER:N	2.49	0.40
1:A:1652:THR:HG21	1:A:2448:THR:CA	2.44	0.40
1:B:1853:ARG:O	1:B:1857:LEU:HG	2.22	0.40
1:B:2551:MET:HE2	1:B:2592:VAL:HG13	2.02	0.40
1:A:2142:PHE:HA	1:A:2145:LEU:HD12	2.04	0.40
1:A:2286:PHE:N	1:A:2287:PRO:CD	2.84	0.40
1:B:1541:ASN:OD1	1:B:1544:ASP:N	2.45	0.40
1:B:1883:TRP:O	1:B:1904:ARG:NH2	2.55	0.40
1:B:2355:SER:HB2	1:B:2360:LEU:HD12	2.04	0.40
1:B:2554:LEU:CD2	1:B:2595:ILE:HG21	2.52	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	1327/2644 (50%)	1274 (96%)	53 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1326/2644 (50%)	1262 (95%)	63 (5%)	1 (0%)	48 80
All	All	2653/5288 (50%)	2536 (96%)	116 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2567	LYS

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	1037/2363 (44%)	1034 (100%)	3 (0%)	91 96
1	B	1075/2363 (46%)	1069 (99%)	6 (1%)	84 92
All	All	2112/4726 (45%)	2103 (100%)	9 (0%)	88 94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2305	SER
1	A	2327	LYS
1	A	2363	ARG
1	B	1466	GLN
1	B	2225	LEU
1	B	2327	LYS
1	B	2374	CYS
1	B	2480	ASN
1	B	2580	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1597	GLN

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Mol	Chain	Res	Type
1	A	1732	GLN
1	A	1862	HIS
1	A	1870	HIS
1	A	1999	HIS
1	A	2077	GLN
1	A	2085	GLN
1	A	2153	HIS
1	A	2307	GLN
1	A	2381	ASN
1	A	2382	ASN
1	A	2408	GLN
1	A	2492	HIS
1	B	1296	ASN
1	B	1344	GLN
1	B	1440	HIS
1	B	1449	HIS
1	B	1520	HIS
1	B	1705	GLN
1	B	1760	HIS
1	B	1762	ASN
1	B	1938	GLN
1	B	1971	GLN
1	B	2039	HIS
1	B	2056	ASN
1	B	2085	GLN
1	B	2382	ASN
1	B	2408	GLN
1	B	2437	HIS
1	B	2480	ASN
1	B	2521	ASN
1	B	2591	HIS
1	B	2600	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	A1EIK	A	2701	-	31,35,35	0.73	1 (3%)	33,53,53	1.28	3 (9%)
2	A1EIK	B	2701	-	31,35,35	0.76	2 (6%)	33,53,53	1.39	3 (9%)

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	A1EIK	A	2701	-	-	0/10/44/44	0/7/6/6
2	A1EIK	B	2701	-	-	0/10/44/44	0/7/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2701	A1EIK	C15-N14	-2.22	1.40	1.44
2	A	2701	A1EIK	C15-N14	-2.07	1.40	1.44
2	B	2701	A1EIK	C11-C10	-2.00	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2701	A1EIK	O4-C3-C2	-5.75	95.25	111.48
2	A	2701	A1EIK	O4-C3-C2	-4.57	98.57	111.48
2	B	2701	A1EIK	C21-C20-C11	-3.15	116.58	119.98
2	A	2701	A1EIK	C21-C20-C11	-3.10	116.63	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2701	A1EIK	C8-N9-C10	-2.18	115.52	118.75
2	A	2701	A1EIK	C8-N9-C10	-2.18	115.53	118.75

There are no chirality outliers.

There are no torsion outliers.

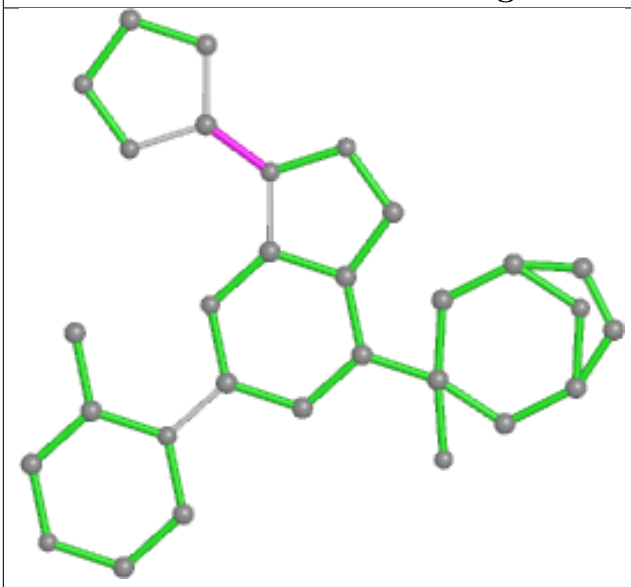
There are no ring outliers.

2 monomers are involved in 4 short contacts:

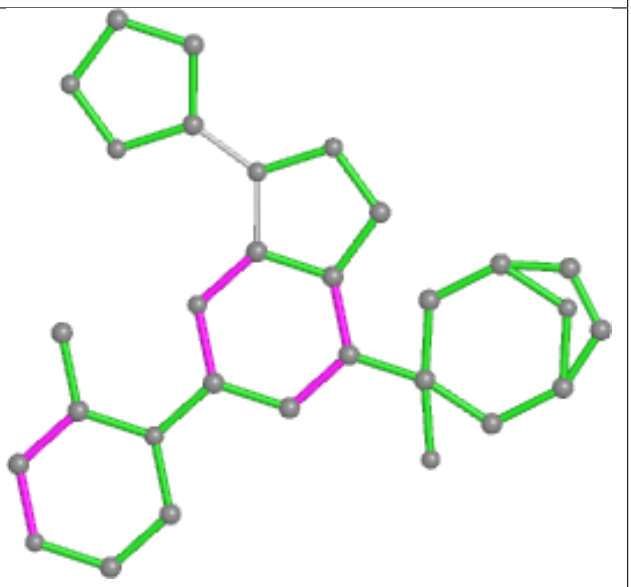
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2701	A1EIK	3	0
2	B	2701	A1EIK	1	0

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.

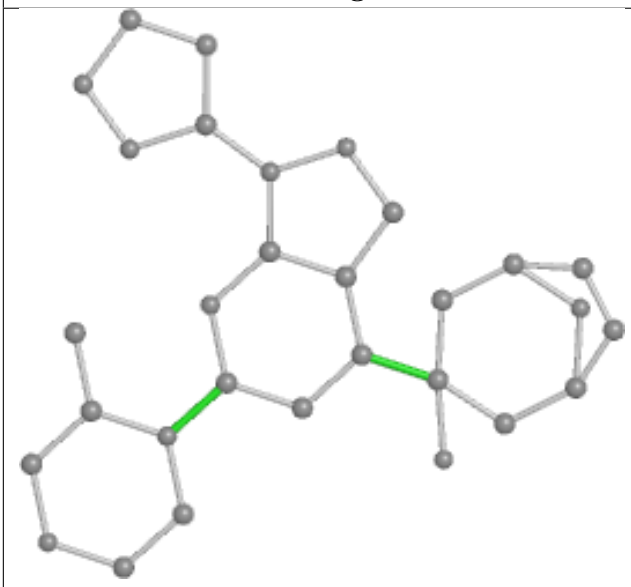
Ligand A1EIK A 2701



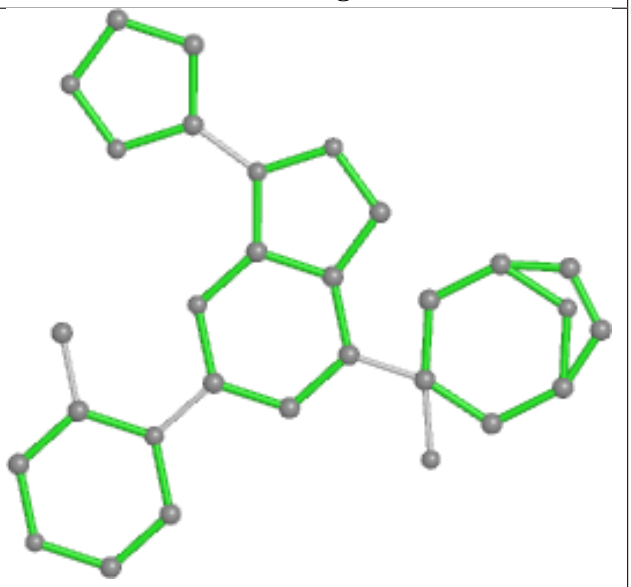
Bond lengths



Bond angles

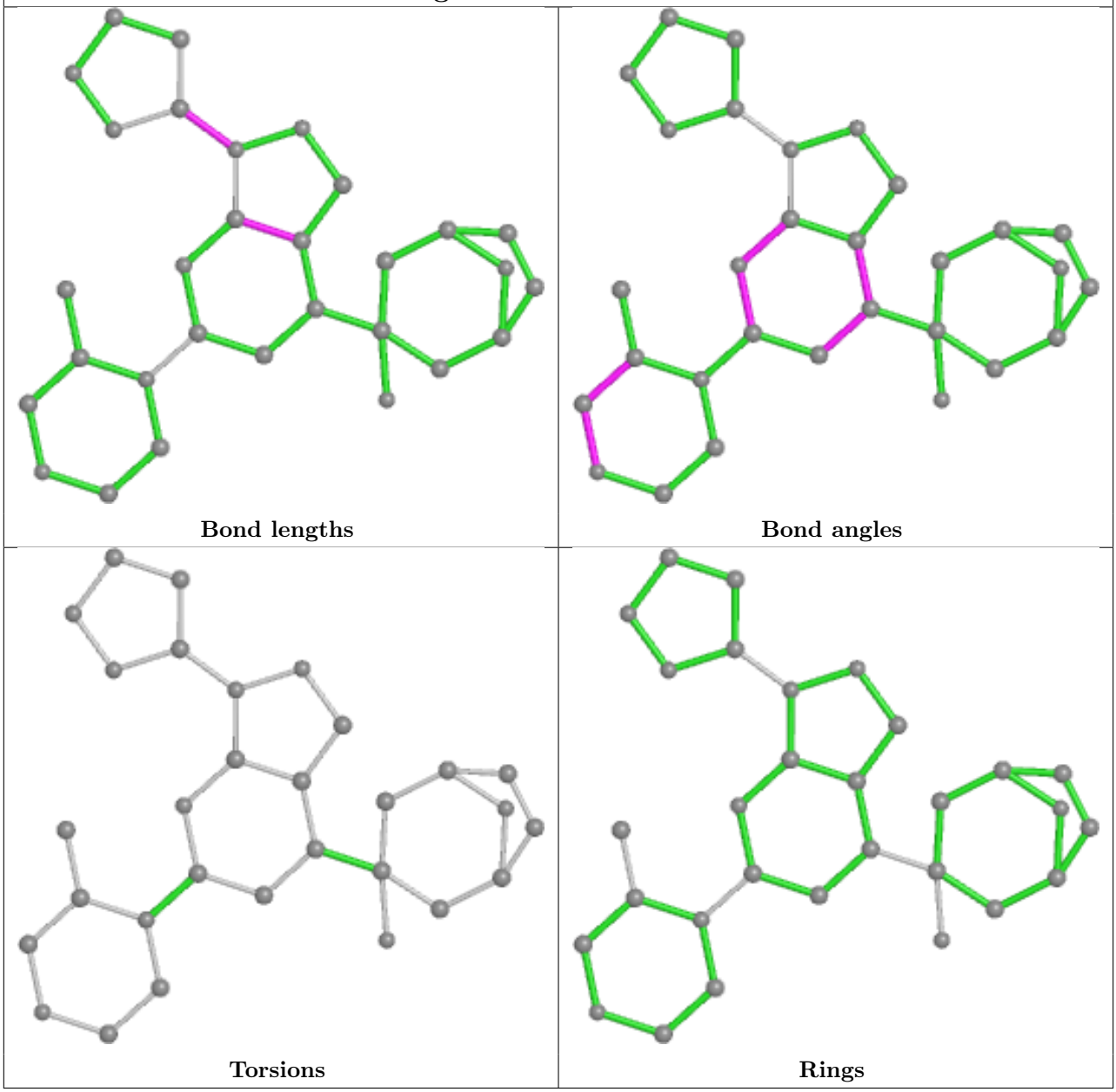


Torsions



Rings

Ligand A1EIK B 2701



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.