



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 12:17 AM JST

PDB ID : 9L40 / pdb_00009L40
EMDB ID : EMD-62801
Title : kinase of ATR bound VE-822 state
Authors : Wang, G.
Deposited on : 2024-12-19
Resolution : 2.87 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

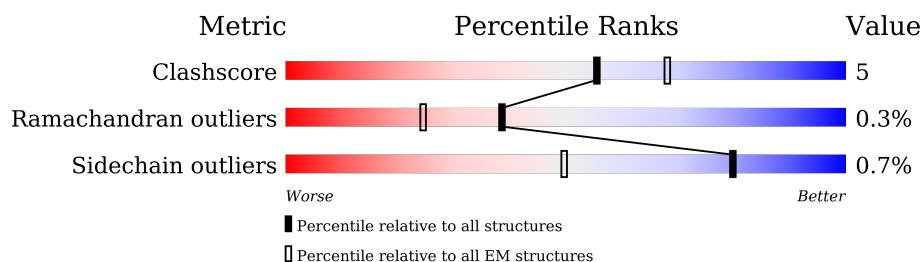
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2644	
1	B	2644	

2 Entry composition [i](#)

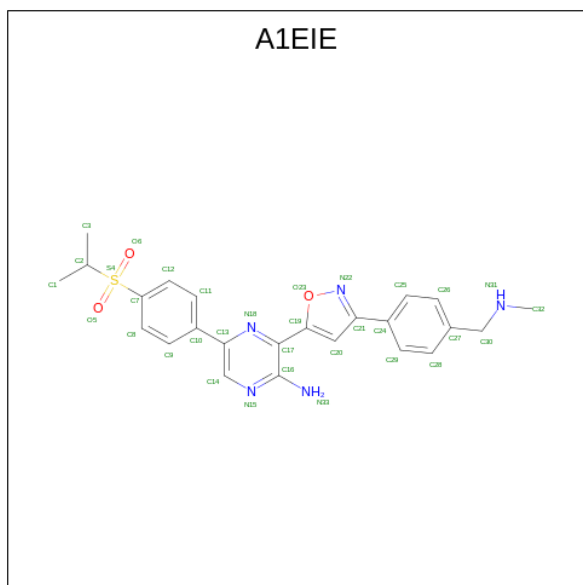
There are 2 unique types of molecules in this entry. The entry contains 35331 atoms, of which 16354 are hydrogens and 0 are deuteriums.

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	1322	Total	C	H	N	O	S	0	0
			17716	5944	8256	1690	1772	54		
1	B	1322	Total	C	H	N	O	S	0	0
			17475	5875	8090	1683	1774	53		

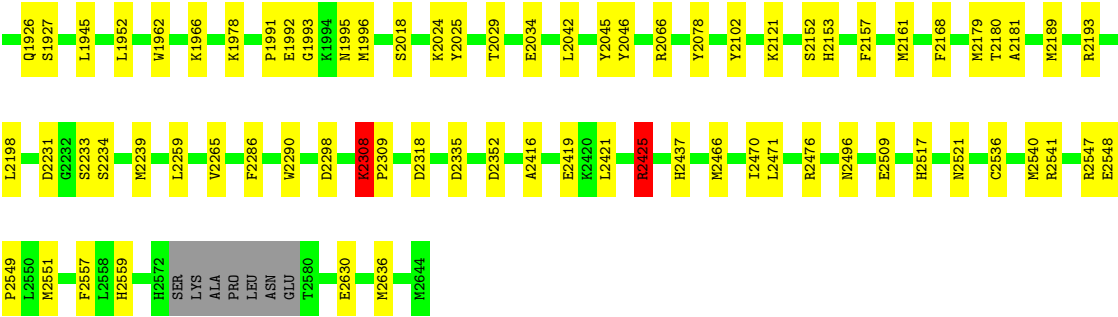
- Molecule 2 is VE-822 (CCD ID: A1EIE) (formula: C₂₄H₂₅N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	A	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	B	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	
2	B	1	Total	C	H	N	O	S	0
			35	24	2	5	3	1	

- Molecule 1: Serine/threonine-protein kinase ATR





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162505	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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EIE

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	0.55	14/9645 (0.1%)	0.61	26/13121 (0.2%)
1	B	0.52	12/9565 (0.1%)	0.59	16/13021 (0.1%)
All	All	0.54	26/19210 (0.1%)	0.60	42/26142 (0.2%)

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	2
1	B	0	4
All	All	0	6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1457	HIS	ND1-CE1	5.27	1.37	1.32
1	A	1558	HIS	ND1-CE1	5.21	1.37	1.32
1	B	1760	HIS	ND1-CE1	5.20	1.37	1.32
1	B	2153	HIS	ND1-CE1	5.20	1.37	1.32
1	A	1302	HIS	ND1-CE1	5.17	1.37	1.32
1	A	2559	HIS	ND1-CE1	5.15	1.37	1.32
1	B	1845	GLN	CD-NE2	-5.15	1.22	1.33
1	A	1531	HIS	ND1-CE1	5.14	1.37	1.32
1	B	1995	ASN	CG-OD1	5.13	1.33	1.23
1	A	1862	HIS	ND1-CE1	5.12	1.37	1.32
1	B	2437	HIS	ND1-CE1	5.11	1.37	1.32
1	A	2437	HIS	ND1-CE1	5.11	1.37	1.32
1	B	1735	HIS	ND1-CE1	5.10	1.37	1.32
1	B	1558	HIS	ND1-CE1	5.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1590	GLN	CD-OE1	5.08	1.33	1.23
1	A	1735	HIS	ND1-CE1	5.08	1.37	1.32
1	A	2517	HIS	ND1-CE1	5.08	1.37	1.32
1	B	1657	HIS	ND1-CE1	5.06	1.37	1.32
1	B	2521	ASN	CG-ND2	-5.05	1.22	1.33
1	B	2559	HIS	ND1-CE1	5.05	1.37	1.32
1	A	1938	GLN	CD-OE1	5.04	1.33	1.23
1	A	2607	ASN	CG-OD1	5.03	1.33	1.23
1	A	2080	ASN	CG-ND2	-5.02	1.22	1.33
1	B	2517	HIS	ND1-CE1	5.01	1.37	1.32
1	B	2559	HIS	CD2-NE2	-5.01	1.32	1.37
1	A	1862	HIS	CD2-NE2	-5.00	1.32	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1477	PRO	N-CA-CB	9.79	109.31	102.65
1	A	1735	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	1457	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	1862	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	B	1760	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	B	2437	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	2559	HIS	CB-CG-CD2	-6.62	122.60	131.20
1	B	2153	HIS	CB-CG-CD2	-6.62	122.60	131.20
1	B	1657	HIS	CB-CG-CD2	-6.61	122.60	131.20
1	B	1735	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	B	1558	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	1302	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	1558	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	2437	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	B	2559	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	1531	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	B	2517	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	2517	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	1855	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	2306	LEU	CA-C-O	-6.19	114.38	121.19
1	B	1760	HIS	CB-CG-ND1	5.75	131.32	122.70
1	A	1735	HIS	CB-CG-ND1	5.74	131.31	122.70
1	A	1862	HIS	CB-CG-ND1	5.73	131.30	122.70
1	A	1457	HIS	CB-CG-ND1	5.71	131.26	122.70
1	B	1558	HIS	CB-CG-ND1	5.71	131.26	122.70
1	B	2437	HIS	CB-CG-ND1	5.71	131.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1558	HIS	CB-CG-ND1	5.70	131.26	122.70
1	A	2437	HIS	CB-CG-ND1	5.69	131.24	122.70
1	B	1735	HIS	CB-CG-ND1	5.68	131.23	122.70
1	A	1302	HIS	CB-CG-ND1	5.68	131.22	122.70
1	A	2559	HIS	CB-CG-ND1	5.68	131.22	122.70
1	B	1657	HIS	CB-CG-ND1	5.65	131.18	122.70
1	A	1531	HIS	CB-CG-ND1	5.65	131.18	122.70
1	B	2153	HIS	CB-CG-ND1	5.65	131.17	122.70
1	B	2559	HIS	CB-CG-ND1	5.64	131.17	122.70
1	B	2517	HIS	CB-CG-ND1	5.51	130.97	122.70
1	A	2517	HIS	CB-CG-ND1	5.51	130.96	122.70
1	A	1477	PRO	CA-C-O	-5.49	114.98	123.16
1	A	1855	HIS	CB-CG-ND1	5.46	130.90	122.70
1	A	2494	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	2328	PRO	N-CA-CB	-5.22	97.77	103.25
1	A	2309	PRO	N-CD-CG	5.01	110.72	103.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1929	ARG	Sidechain
1	A	2425	ARG	Sidechain
1	B	1566	THR	Peptide
1	B	1952	LEU	Peptide
1	B	2425	ARG	Sidechain
1	B	2476	ARG	Sidechain

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	9460	8256	8273	85	0
1	B	9385	8090	8122	83	0
2	A	66	4	0	1	0
2	B	66	4	0	2	0
All	All	18977	16354	16395	169	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 5.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1455:GLU:O	1:B:1458:LEU:N	2.02	0.92
1:B:1354:CYS:HA	1:B:1357:CYS:SG	2.16	0.86
1:B:1573:LEU:O	1:B:1577:SER:OG	1.99	0.81
1:A:1403:ALA:O	1:A:1407:TYR:N	2.16	0.79
1:B:1945:LEU:HG	2:B:2702:A1EIE:C32	2.13	0.78
1:B:2425:ARG:NH2	1:B:2630:GLU:OE2	2.16	0.78
1:B:1588:LEU:CB	1:B:1633:LEU:HD21	2.18	0.73
1:B:1451:ARG:HA	1:B:1454:LEU:CB	2.21	0.70
1:B:1402:ARG:O	1:B:1406:ALA:HB2	1.95	0.66
1:B:1991:PRO:HA	1:B:1996:MET:HE3	1.81	0.61
1:B:1553:MET:HE1	1:B:1637:PRO:HD2	1.82	0.60
1:A:1448:GLU:HA	1:A:1451:ARG:CB	2.31	0.60
1:A:2303:LEU:HD21	1:A:2311:LYS:HD3	1.84	0.60
1:A:2169:LEU:HD22	1:A:2204:MET:HE2	1.84	0.59
1:A:2466:MET:HE3	1:A:2536:CYS:SG	2.43	0.58
1:A:1441:GLN:HA	1:A:1444:ARG:CB	2.34	0.58
1:A:1784:TRP:CD1	1:A:1812:LYS:HZ2	2.22	0.57
1:B:1715:LEU:HA	1:B:1718:ALA:HB3	1.86	0.57
1:B:1447:PRO:O	1:B:1451:ARG:N	2.37	0.56
1:B:2466:MET:HE3	1:B:2536:CYS:SG	2.46	0.56
1:A:1403:ALA:HA	1:A:1406:ALA:HB3	1.87	0.55
1:A:1438:PRO:O	1:A:1442:LEU:HD23	2.06	0.54
1:A:2236:THR:OG1	1:A:2299:MET:HE3	2.08	0.53
1:A:1390:SER:CB	1:A:1442:LEU:HG	2.39	0.53
1:B:2466:MET:SD	1:B:2540:MET:HE2	2.49	0.53
1:A:1486:ASN:N	1:A:1489:GLU:OE2	2.42	0.53
1:A:1429:ASP:CB	1:A:1439:GLY:HA3	2.39	0.52
1:B:1447:PRO:O	1:B:1450:VAL:N	2.42	0.52
1:A:2306:LEU:O	1:A:2309:PRO:HD3	2.10	0.52
1:B:1595:LYS:O	1:B:1598:ALA:HB3	2.11	0.51
2:A:2701:A1EIE:C32	2:A:2701:A1EIE:C26	2.89	0.51
1:A:1447:PRO:O	1:A:1449:HIS:N	2.44	0.51
1:A:1437:GLY:O	1:A:1440:HIS:CB	2.60	0.50
1:A:1580:THR:O	1:A:1584:MET:HE3	2.12	0.49
1:A:1580:THR:C	1:A:1584:MET:HE3	2.37	0.49
1:A:2515:LEU:HD11	1:A:2523:MET:HE1	1.94	0.49
1:A:2022:MET:HE3	1:A:2046:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2421:LEU:HG	1:B:2425:ARG:HD2	1.95	0.49
1:B:1455:GLU:O	1:B:1456:PRO:C	2.55	0.49
1:B:2168:PHE:CD2	1:B:2179:MET:HE2	2.47	0.49
1:B:2547:ARG:O	1:B:2551:MET:HB2	2.13	0.49
1:A:2303:LEU:HD21	1:A:2311:LYS:CD	2.42	0.49
1:B:1354:CYS:HA	1:B:1357:CYS:CB	2.42	0.49
1:A:1478:ILE:O	1:A:1479:TYR:C	2.56	0.49
1:B:1992:GLU:O	1:B:1993:GLY:C	2.55	0.49
1:A:1448:GLU:O	1:A:1448:GLU:HG2	2.12	0.48
1:B:1478:ILE:O	1:B:1484:GLY:HA3	2.13	0.48
1:B:1455:GLU:O	1:B:1457:HIS:N	2.47	0.47
1:A:1521:ASP:O	1:A:1525:THR:OG1	2.28	0.47
1:A:2217:ARG:O	1:A:2220:ASP:OD2	2.32	0.47
1:B:2548:GLU:HB2	1:B:2549:PRO:HD3	1.96	0.47
1:A:2400:TYR:O	1:A:2431:ARG:NH1	2.48	0.46
1:B:2239:MET:HE3	1:B:2239:MET:HB3	1.81	0.46
1:A:1517:MET:O	1:A:1521:ASP:N	2.48	0.46
1:B:1354:CYS:CA	1:B:1357:CYS:SG	2.96	0.46
1:B:2233:SER:O	1:B:2234:SER:C	2.59	0.46
1:A:1442:LEU:HA	1:A:1442:LEU:HD13	1.58	0.46
1:B:2102:TYR:CD2	1:B:2152:SER:HB3	2.51	0.46
1:A:2063:ASP:N	1:A:2118:ASP:OD1	2.49	0.45
1:A:1403:ALA:O	1:A:1406:ALA:N	2.49	0.45
1:B:2509:GLU:HG2	1:B:2636:MET:HE1	1.99	0.45
1:A:1911:ASN:O	1:A:1916:TYR:CE2	2.69	0.45
1:B:1736:TYR:O	1:B:1740:VAL:HG23	2.17	0.45
1:B:2102:TYR:CE2	1:B:2152:SER:HB3	2.52	0.45
1:A:2429:LEU:HA	1:A:2429:LEU:HD23	1.65	0.45
1:B:1567:GLN:O	1:B:1571:SER:N	2.46	0.45
1:B:2421:LEU:HD21	1:B:2425:ARG:HH11	1.82	0.45
1:A:2109:ARG:N	1:A:2109:ARG:HD3	2.32	0.44
1:B:1498:LEU:O	1:B:1501:LYS:N	2.50	0.44
1:A:2306:LEU:H	1:A:2306:LEU:HD22	1.82	0.44
1:B:1425:LEU:HA	1:B:1428:TYR:O	2.16	0.44
1:B:2318:ASP:N	1:B:2318:ASP:OD1	2.48	0.44
1:B:2470:ILE:HG13	1:B:2471:LEU:N	2.31	0.44
1:B:2496:ASN:C	1:B:2496:ASN:HD22	2.26	0.44
1:B:2157:PHE:CE2	1:B:2161:MET:HE3	2.52	0.44
1:A:1414:GLN:O	1:A:1415:ASP:C	2.61	0.44
1:A:2181:ALA:HB2	1:A:2369:PRO:O	2.17	0.44
1:B:2168:PHE:HD2	1:B:2179:MET:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1996:MET:HE3	1:A:2032:LEU:HD23	1.99	0.44
1:B:1639:ASP:OD1	1:B:1640:THR:N	2.50	0.44
1:B:2231:ASP:O	1:B:2234:SER:OG	2.29	0.44
1:A:2134:ALA:HB2	1:A:2280:HIS:O	2.18	0.44
1:B:1402:ARG:O	1:B:1406:ALA:CB	2.66	0.44
1:A:1512:THR:O	1:A:1513:CYS:C	2.61	0.43
1:B:1463:LYS:O	1:B:1464:SER:C	2.60	0.43
1:B:1713:GLY:C	1:B:1714:LEU:HD22	2.42	0.43
1:A:1442:LEU:HD22	1:A:1442:LEU:N	2.32	0.43
1:B:1376:THR:O	1:B:1376:THR:HG23	2.17	0.43
1:A:1437:GLY:O	1:A:1438:PRO:C	2.62	0.43
1:B:1709:HIS:HB3	1:B:1718:ALA:HB2	1.99	0.43
1:A:1307:LEU:O	1:A:1311:LEU:HG	2.18	0.43
1:B:2025:TYR:O	1:B:2029:THR:HG23	2.18	0.43
1:B:2180:THR:HG23	1:B:2181:ALA:N	2.33	0.43
1:A:2636:MET:HE3	1:A:2636:MET:HB3	1.82	0.43
1:B:1813:LYS:O	1:B:1814:ARG:C	2.62	0.43
1:A:1327:THR:HG23	1:A:1368:ARG:O	2.19	0.42
1:A:2190:ARG:NH1	1:A:2581:GLY:O	2.50	0.42
1:A:2278:ALA:O	1:A:2283:HIS:HB2	2.19	0.42
1:B:1804:LEU:HD12	1:B:1804:LEU:HA	1.87	0.42
1:A:1539:GLY:O	1:A:1540:CYS:SG	2.75	0.42
1:A:1886:ARG:HA	1:A:1889:MET:HE2	2.01	0.42
1:A:2306:LEU:O	1:A:2309:PRO:CD	2.67	0.42
1:B:2239:MET:N	1:B:2298:ASP:O	2.37	0.42
1:A:2070:LEU:HD23	1:A:2070:LEU:C	2.45	0.42
1:B:2308:LYS:O	1:B:2309:PRO:C	2.63	0.42
1:A:2005:LEU:HD12	1:A:2005:LEU:HA	1.83	0.42
1:B:2416:ALA:N	1:B:2419:GLU:OE1	2.49	0.42
1:A:1890:THR:HG22	1:A:1891:GLN:N	2.35	0.42
1:A:2269:THR:O	1:A:2283:HIS:NE2	2.44	0.42
1:B:2024:LYS:HB2	1:B:2024:LYS:HE2	1.89	0.42
1:A:1821:ASP:O	1:A:1825:LEU:HD13	2.19	0.42
1:A:2064:LEU:HD23	1:A:2064:LEU:HA	1.81	0.42
1:A:2425:ARG:HH21	1:A:2630:GLU:HB2	1.84	0.42
1:A:1714:LEU:HD12	1:A:1714:LEU:N	2.34	0.42
1:A:1855:HIS:C	1:A:1855:HIS:CD2	2.97	0.42
1:A:2022:MET:HE3	1:A:2046:TYR:CE2	2.55	0.42
1:A:2084:TYR:O	1:A:2088:PRO:HG2	2.20	0.42
1:A:2423:VAL:HA	1:A:2427:PHE:CD2	2.55	0.42
1:A:1362:GLY:HA3	1:A:1889:MET:HE1	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2223:LEU:HD12	1:A:2223:LEU:HA	1.90	0.41
1:B:1629:VAL:O	1:B:1633:LEU:HG	2.20	0.41
1:B:2042:LEU:HD11	1:B:2046:TYR:CE1	2.55	0.41
1:A:1341:LYS:HA	1:A:1344:GLN:OE1	2.20	0.41
1:A:1352:LEU:O	1:A:1356:GLU:HG3	2.20	0.41
1:B:2286:PHE:HB2	1:B:2290:TRP:HZ2	1.85	0.41
1:A:1537:LEU:C	1:A:1539:GLY:H	2.28	0.41
1:B:1905:ARG:HH12	1:B:1927:SER:HG	1.64	0.41
1:B:2034:GLU:O	1:B:2078:TYR:HB3	2.20	0.41
1:A:2610:THR:O	1:A:2610:THR:HG23	2.20	0.41
1:B:1912:LYS:HA	1:B:1912:LYS:HD3	1.63	0.41
1:B:2066:ARG:HD3	1:B:2121:LYS:HB3	2.02	0.41
1:B:2259:LEU:HD21	1:B:2265:VAL:CG2	2.50	0.41
1:A:2077:GLN:HE22	1:A:2132:TYR:HD2	1.68	0.41
1:B:1331:ILE:HD12	1:B:1331:ILE:HA	1.91	0.41
1:B:1478:ILE:O	1:B:1484:GLY:N	2.53	0.41
1:B:2018:SER:HA	1:B:2045:TYR:OH	2.20	0.41
1:A:1916:TYR:O	1:A:1920:VAL:HG23	2.21	0.41
1:A:2303:LEU:HD11	1:A:2311:LYS:HD2	2.01	0.41
1:B:1349:GLN:O	1:B:1353:LEU:HG	2.20	0.41
1:B:1962:TRP:CZ2	1:B:1966:LYS:HD2	2.56	0.41
1:B:2198:LEU:HD23	1:B:2198:LEU:HA	1.93	0.41
1:B:2557:PHE:CD1	1:B:2557:PHE:O	2.73	0.41
1:A:1815:ASP:C	1:A:1815:ASP:OD2	2.64	0.41
1:B:1744:LEU:HD21	1:B:1776:GLU:CD	2.45	0.41
1:B:1922:GLU:O	1:B:1926:GLN:HG3	2.20	0.41
1:A:2329:LYS:O	1:A:2330:ASP:OD1	2.39	0.41
1:B:1354:CYS:CB	1:B:1357:CYS:SG	3.09	0.41
1:B:1945:LEU:CG	2:B:2702:A1EIE:C32	2.93	0.41
1:A:1510:ILE:HA	1:A:1513:CYS:CB	2.51	0.40
1:A:2546:GLN:O	1:A:2550:LEU:HG	2.21	0.40
1:A:2554:LEU:HD23	1:A:2554:LEU:HA	1.93	0.40
1:B:1712:LEU:HD12	1:B:1712:LEU:N	2.36	0.40
1:B:2189:MET:HE3	1:B:2193:ARG:NH2	2.36	0.40
1:B:1712:LEU:O	1:B:1714:LEU:HD23	2.21	0.40
1:B:1895:ARG:HD3	1:B:1895:ARG:N	2.36	0.40
1:A:1495:ALA:HB2	1:A:1529:LEU:HD21	2.02	0.40
1:A:1992:GLU:O	1:A:1993:GLY:C	2.65	0.40
1:A:2165:ALA:O	1:A:2169:LEU:HD13	2.22	0.40
1:A:2259:LEU:HD21	1:A:2265:VAL:HB	2.04	0.40
1:A:2561:PRO:CB	1:A:2582:GLU:HG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1364:ILE:O	1:B:1365:ASP:C	2.64	0.40
1:A:1481:SER:O	1:A:1482:LYS:C	2.64	0.40
1:A:2058:MET:HE2	1:A:2058:MET:HB3	1.92	0.40
1:A:2155:GLU:OE1	1:A:2155:GLU:N	2.47	0.40
1:B:1455:GLU:HA	1:B:1458:LEU:CB	2.52	0.40
1:B:1580:THR:O	1:B:1583:SER:HB2	2.21	0.40
1:B:2352:ASP:OD2	1:B:2541:ARG:NH1	2.51	0.40
1:A:1762:ASN:OD1	1:A:1763:ARG:N	2.55	0.40
1:A:2303:LEU:HD12	1:A:2309:PRO:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1310/2644 (50%)	1233 (94%)	72 (6%)	5 (0%)	30	58
1	B	1312/2644 (50%)	1249 (95%)	61 (5%)	2 (0%)	44	71
All	All	2622/5288 (50%)	2482 (95%)	133 (5%)	7 (0%)	38	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2307	GLN
1	B	2308	LYS
1	A	1478	ILE
1	A	2305	SER
1	A	2328	PRO
1	B	1476	LYS
1	A	2309	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	823/2363 (35%)	816 (99%)	7 (1%)	75	91
1	B	808/2363 (34%)	804 (100%)	4 (0%)	86	95
All	All	1631/4726 (34%)	1620 (99%)	11 (1%)	80	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1354	CYS
1	A	1929	ARG
1	A	2306	LEU
1	A	2308	LYS
1	A	2310	LYS
1	A	2328	PRO
1	A	2564	GLU
1	B	1978	LYS
1	B	2308	LYS
1	B	2335	ASP
1	B	2425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1672	HIS
1	A	1946	ASN
1	A	1970	HIS
1	A	1999	HIS
1	A	2227	ASN
1	A	2621	HIS
1	A	2631	ASN
1	B	1891	GLN
1	B	1970	HIS
1	B	2114	GLN
1	B	2199	ASN

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Mol	Chain	Res	Type
1	B	2307	GLN
1	B	2437	HIS
1	B	2621	HIS

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](#)

4 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	A1EIE	A	2702	-	33,36,36	0.64	1 (3%)	43,52,52	0.72	2 (4%)
2	A1EIE	B	2702	-	33,36,36	0.64	2 (6%)	43,52,52	0.61	1 (2%)
2	A1EIE	A	2701	-	33,36,36	0.66	2 (6%)	43,52,52	0.75	1 (2%)
2	A1EIE	B	2701	-	33,36,36	0.62	1 (3%)	43,52,52	0.67	1 (2%)

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	A1EIE	A	2702	-	-	7/22/27/27	0/4/4/4
2	A1EIE	B	2702	-	-	8/22/27/27	0/4/4/4
2	A1EIE	A	2701	-	-	6/22/27/27	0/4/4/4
2	A1EIE	B	2701	-	-	5/22/27/27	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2701	A1EIE	C30-N31	2.22	1.49	1.46
2	B	2702	A1EIE	C17-C16	-2.22	1.42	1.45
2	A	2702	A1EIE	C30-N31	2.12	1.49	1.46
2	B	2701	A1EIE	C30-N31	2.09	1.49	1.46
2	B	2702	A1EIE	C30-N31	2.07	1.49	1.46
2	A	2701	A1EIE	C17-C16	-2.05	1.42	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2701	A1EIE	C19-C17-N18	-3.41	108.74	115.09
2	B	2701	A1EIE	C19-C17-N18	-2.63	110.21	115.09
2	A	2702	A1EIE	C19-C17-N18	-2.25	110.92	115.09
2	A	2702	A1EIE	C20-C19-C17	2.04	135.34	129.21
2	B	2702	A1EIE	C16-C17-N18	2.04	121.30	119.92

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2701	A1EIE	C1-C2-S4-C7
2	A	2701	A1EIE	C1-C2-S4-O5
2	A	2701	A1EIE	C1-C2-S4-O6
2	A	2701	A1EIE	C3-C2-S4-C7
2	A	2701	A1EIE	C3-C2-S4-O5
2	A	2701	A1EIE	C3-C2-S4-O6
2	A	2702	A1EIE	N22-C21-C24-C25
2	A	2702	A1EIE	C1-C2-S4-O6
2	B	2701	A1EIE	C1-C2-S4-C7
2	B	2701	A1EIE	C1-C2-S4-O5
2	B	2701	A1EIE	C1-C2-S4-O6
2	B	2701	A1EIE	C3-C2-S4-O6
2	B	2702	A1EIE	C1-C2-S4-C7

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Mol	Chain	Res	Type	Atoms
2	B	2702	A1EIE	C1-C2-S4-O5
2	B	2702	A1EIE	C1-C2-S4-O6
2	B	2702	A1EIE	C3-C2-S4-C7
2	B	2702	A1EIE	C3-C2-S4-O5
2	B	2702	A1EIE	C3-C2-S4-O6
2	A	2702	A1EIE	C8-C7-S4-O6
2	A	2702	A1EIE	C12-C7-S4-O6
2	A	2702	A1EIE	C12-C7-S4-C2
2	A	2702	A1EIE	C8-C7-S4-C2
2	A	2702	A1EIE	C3-C2-S4-O6
2	B	2701	A1EIE	C3-C2-S4-C7
2	B	2702	A1EIE	C12-C7-S4-O6
2	B	2702	A1EIE	C8-C7-S4-O6

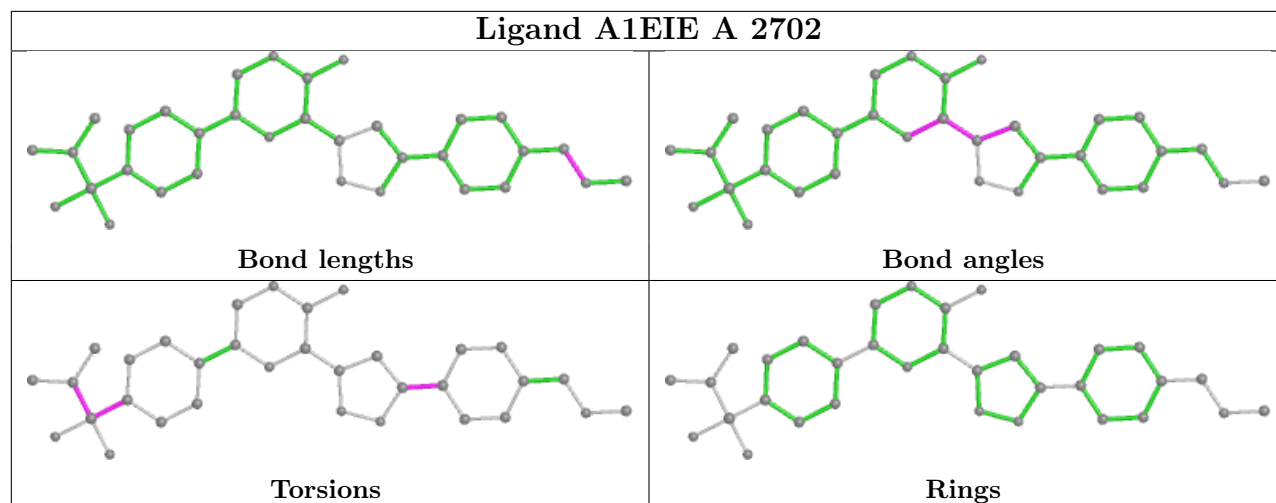
There are no ring outliers.

2 monomers are involved in 3 short contacts:

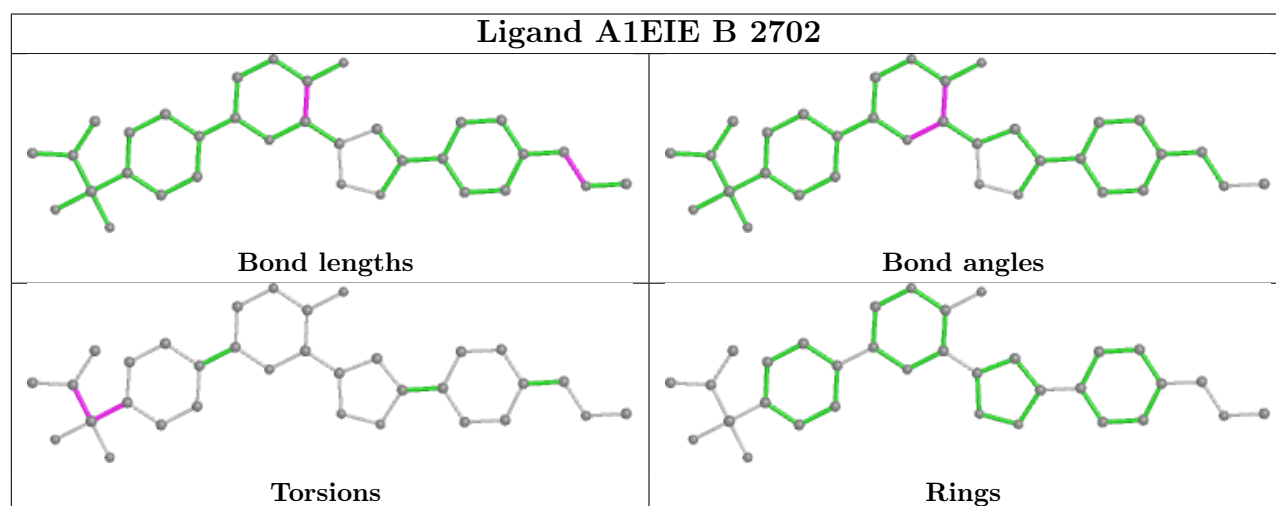
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2702	A1EIE	2	0
2	A	2701	A1EIE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

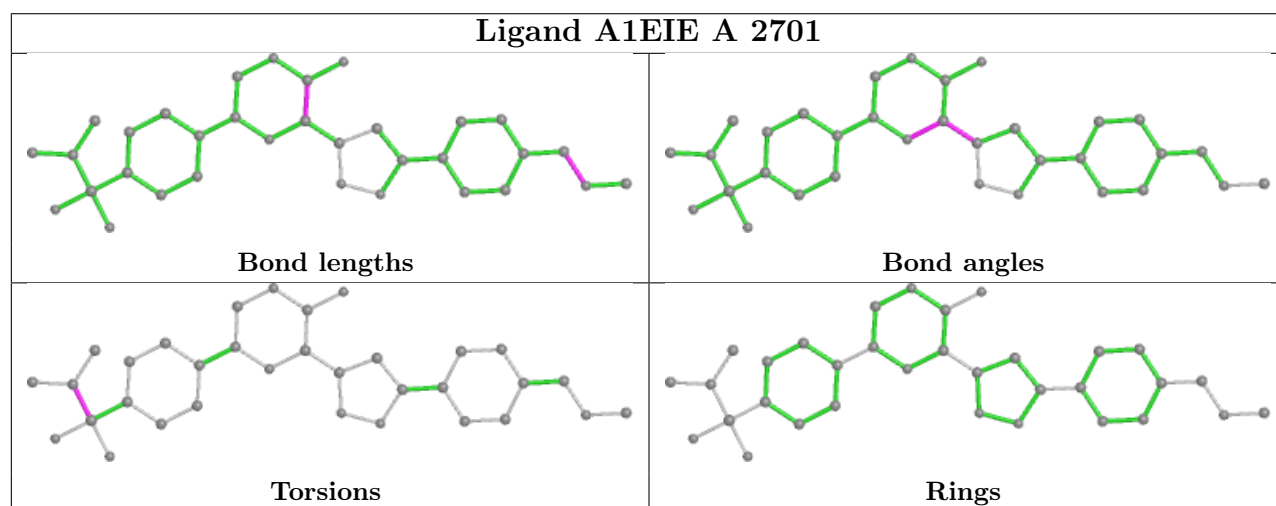
Ligand A1EIE A 2702

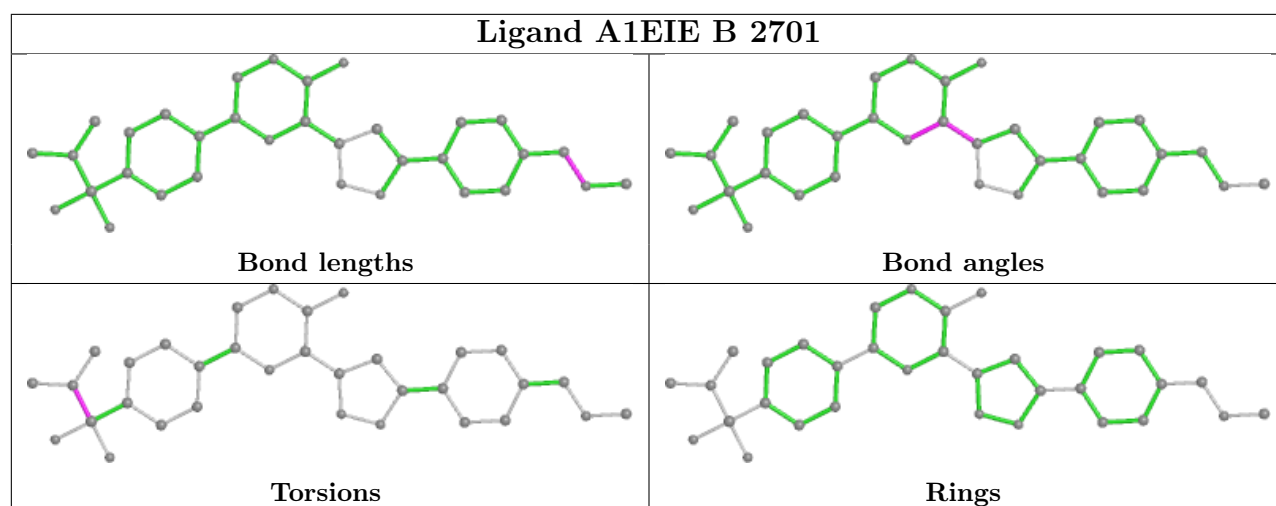


Ligand A1EIE B 2702



Ligand A1EIE A 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.