



wwPDB EM Validation Summary Report ⓘ

May 25, 2025 – 12:33 AM JST

PDB ID : 9L4D / pdb_0000914d
EMDB ID : EMD-62811
Title : ATR-ATRIP bound with RP-3500
Authors : Wang, G.
Deposited on : 2024-12-20
Resolution : 3.79 Å (reported)

This is a wwPDB EM Validation Summary 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

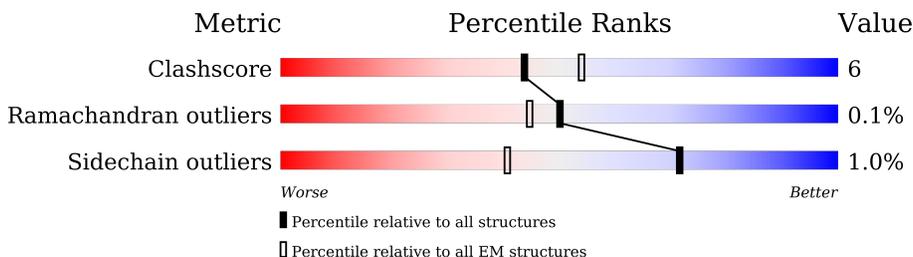
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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	2637	
1	B	2637	
2	C	491	
2	D	491	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 67221 atoms, of which 29861 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.

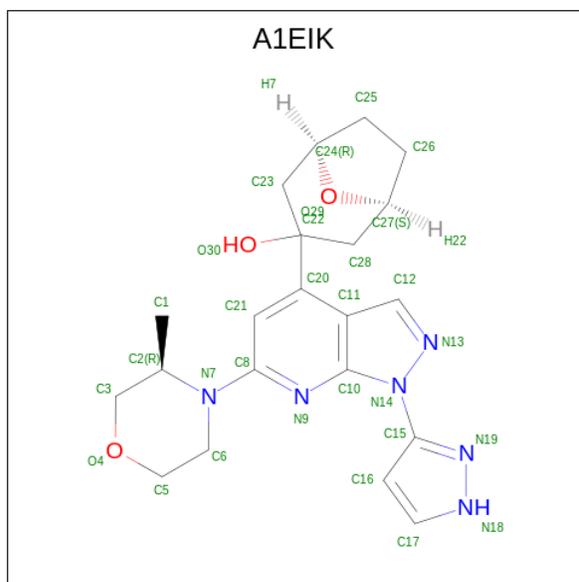
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2473	Total	C	H	N	O	S	0	0
			26772	9217	11475	2847	3181	52		
1	B	2497	Total	C	H	N	O	S	0	0
			31311	10642	14272	3025	3281	91		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	D	382	Total	C	H	N	O	S	0	0
			4498	1510	2026	462	485	15		
2	C	382	Total	C	H	N	O	S	0	0
			4579	1521	2088	461	485	24		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			30	21	6	3	
3	B	1	Total	C	N	O	0
			30	21	6	3	

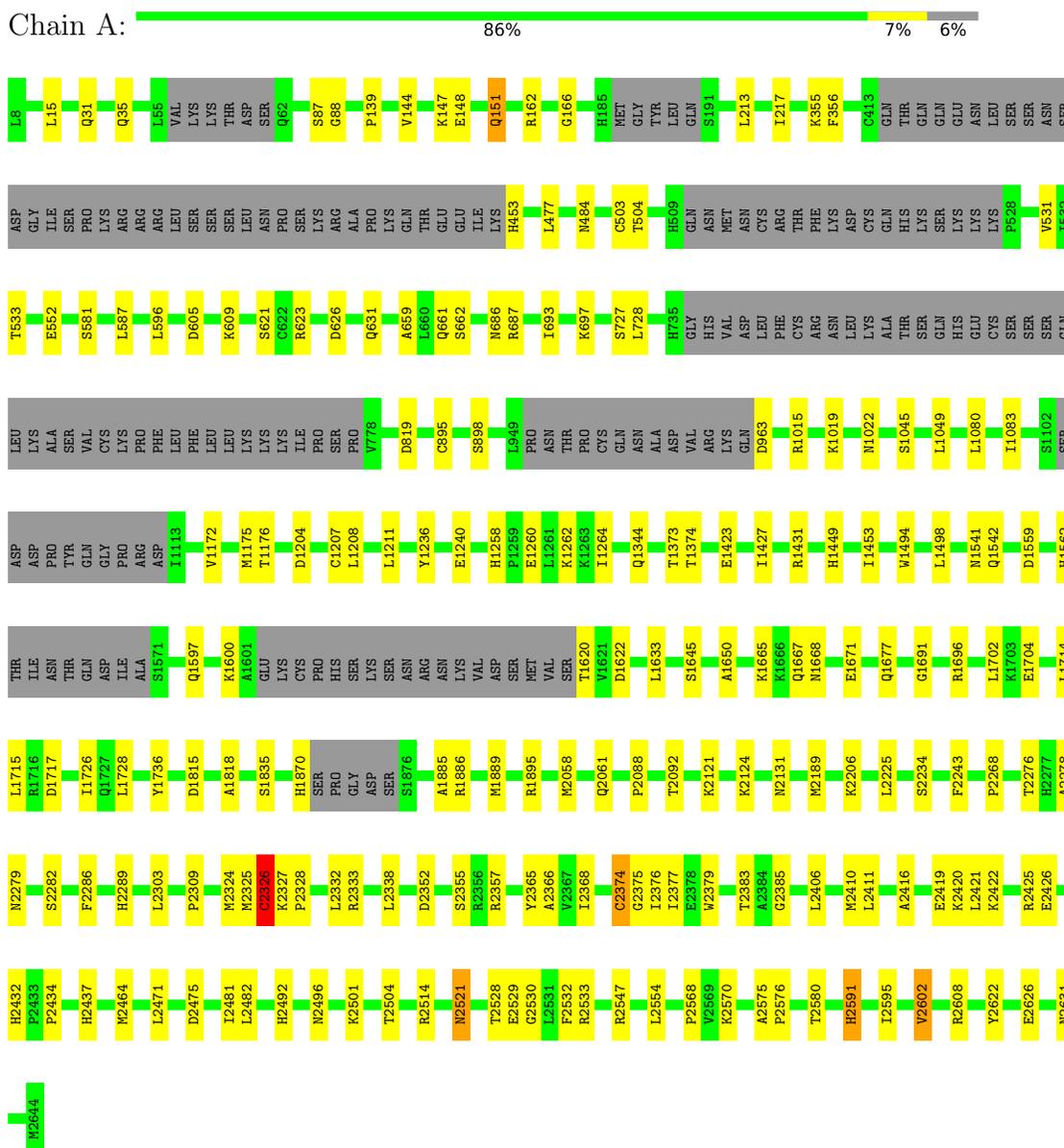
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	

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.

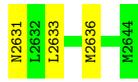
- Molecule 1: Serine/threonine-protein kinase ATR



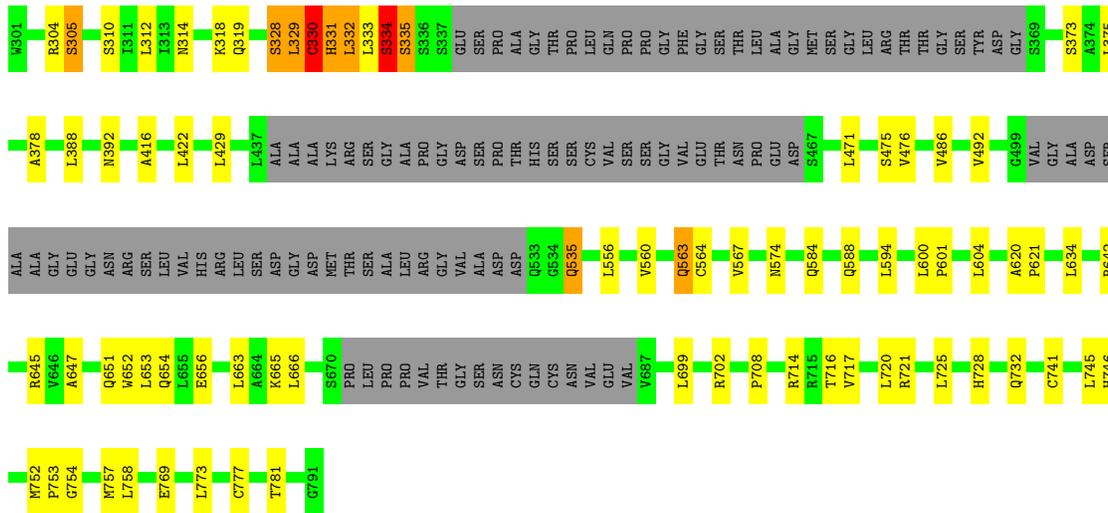
- Molecule 1: Serine/threonine-protein kinase ATR

Chain B: 81% 13% 5%

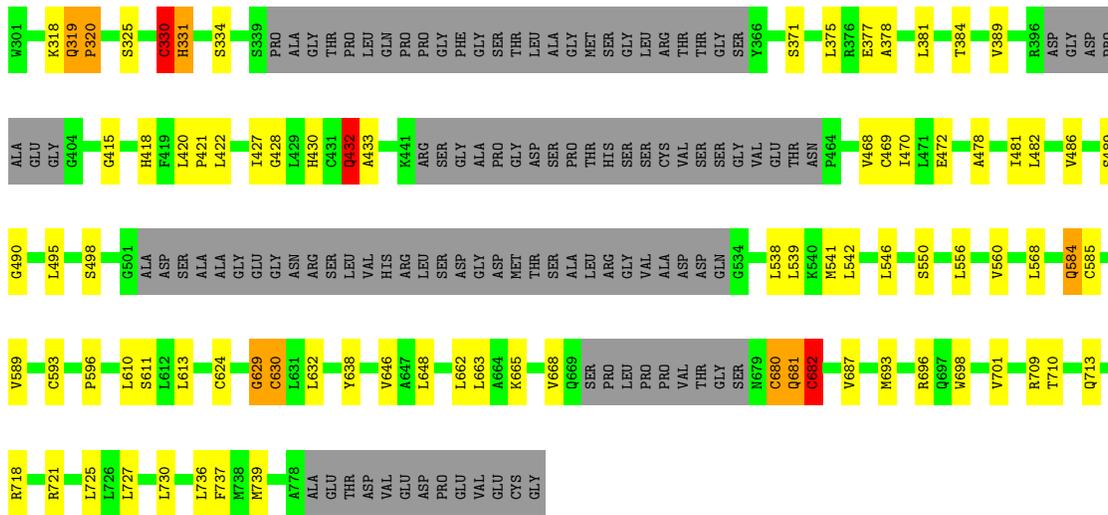
LEU	ALA	S10	M11	I12	P13	R16	P23	Y26	K32	I36	V51	A52	V53	E54	L55	VAL	LYS	LYS	THR	ASP	SER	GLN	PRO	T64	D70	Q73	K77	N85	S89	H90	E91	A92	K93	N101	R106	R109	S115	C124	E125	F134	K135							
I141	F142	K147	E282	D284	T285	D286	S296	M171	P172	F178	D183	HIS	NET	GLY	TYR	LEU	GLN	SER	A192	E203	V207	L210	L213	L217	A218	I219	V220	F221	F222	R223	A364	L365	Q366	C234	I244	L247	S250	F251	L255	F256	G124	L261	P262	L276				
H279	L280	V281	M283	D284	T285	D286	S296	K300	T301	F304	F305	E306	Y317	M320	L321	L322	E323	V327	D340	L341	L342	F343	I219	Y352	F356	A364	L365	Q366	R373	K377	Y382	E386	Q414	THR	L255	F256	G124	L261	P262	ASN	LEU	SER						
SER	ASN	ASP	ASP	ILE	SER	PRO	LYS	ARG	ARG	ARG	LEU	SER	PRO	LYS	ARG	ALA	PRO	LYS	GLN	THR	THR	GLU	GLU	L451	T504	M512	ASN	CYS	ARG	THR	PHE	LYS	ASP	CYS	GLN	HIS	LYS	SER	LYS	LYS	PRO	S529	V554	J555	K556	L557	Y656	L660
V688	V703	L848	K705	E706	L714	T717	G720	L724	S726	H735	G736	V738	L745	A747	L748	S749	Q750	H751	A760	S761	V762	C763	L767	I774	H787	F795	V802	G807	M813	D817	V820	H830	L831	L832	G840	A1101	SER	SER	ASP	ASP	THR	TYR	GLN					
K843	E844	V847	L848	R849	E852	T855	Q858	T868	L869	A879	L890	L893	A901	S904	P952	A948	PRO	ASN	THR	THR	CYS	C763	L767	I774	H787	F795	V802	G807	M813	D817	V820	H830	L831	L832	G840	A1101	SER	SER	ASP	ASP	THR	TYR	GLN					
H109	P110	R111	L1138	SER	SER	SER	VAL	GLY	ILE	GLU	ASP	K1148	K1149	M1150	A1151	L1152	N1153	G1163	H1166	V1170	K1173	S749	Q750	H751	F1188	P1189	E1190	M1191	C1192	C1193	R1194	D1197	L1211	L1212	S1213	I1216	P1221	I1225	G1354	F1234	E1356	I1239	R1242	D1243				
A1244	F1248	K1263	I1264	V1267	R1272	LYS	GLU	THR	SER	GLU	THR	K1148	K1149	M1150	A1151	L1281	S1288	V1297	R1300	I1301	L1307	E1309	T1310	L1311	F1188	P1189	E1190	M1191	C1192	C1193	R1194	D1197	L1211	L1212	S1213	I1216	P1221	I1225	G1354	F1234	E1356	I1239	R1242	D1243				
A1403	A1406	R1431	GLU	MET	GLU	THR	ASN	PRO	GLY	H1440	S1481	K1482	L1483	M1518	T1525	L1533	L1537	Q1542	Q1546	D1559	H1562	T1563	A1570	L1573	V1581	M1584	T1589	K1595	L1599	K1600	A1601	GLU	LYS	CYS	PRO	HIS	SER	LYS	SER									
ASN	ARG	ASN	LYS	VAL	ASP	MET	VAL	S1619	Y1623	F1632	L1635	D1639	M1656	H1657	F1658	I1662	N1668	E1671	F1675	K1678	L1702	I1706	L1712	Y1722	V1739	M1757	H1760	T1767	W1784	V1787	T1798	T1799	W1800	R1803	I1831	A1831												
R1853	M1856	H1862	K1865	Q1869	H1870	SER	PRO	GLY	ASP	S1876	Q1877	L1881	R1886	M1889	P1889	K1912	M1924	A1947	G1948	R1951	L1955	C1983	G1993	M1996	L2005	M2019	M2022	W2035	E2036	D2037	L2042	W2046	M2052															
M2058	Q2061	D2063	F2072	S2075	L2076	S2086	M2087	L2119	N2123	Y2136	L2139	D2154	F2157	Q2174	V2182	S2183	K2184	S2185	R2193	C2194	G2213	R2217	L2218	T2219	D2220	K2221	S2238	H2242	K2248	L2259	M2266	T2269	L2270	P2271	H2280	A2281												
S2282	H2283	M2290	L2303	M2304	S2305	Q2307	K2308	P2309	M2310	K2311	M2324	M2325	C2326	K2327	P2328	K2329	L2332	R2333	K2334	D2335	E2340	S2343	R2366	R2367	G2375	L2376	L2377	E2378	M2379	V2380	T2383	A2384	C2385	P2388	L2389	L2421	P2434	E2436	W2439	F2440	L2441	Y2457						
T2461	M2464	S2465	M2466	V2467	L2471	T2481	L2482	H2492	C2497	L2498	G2502	V2511	P2512	F2513	R2514	L2515	T2516	M2519	V2520	M2521	E2529	R2533	T2539	M2540	M2543	E2548	P2549	L2550	M2551	V2563	K2567	T2580	G2581	E2582	M2585	E2586	K2587	A2588	V2592									



• Molecule 2: ATR-interacting protein



• Molecule 2: ATR-interacting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77631	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 (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: ZN, 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	0.34	10/15382 (0.1%)	0.50	16/21057 (0.1%)
1	B	0.38	6/17289 (0.0%)	0.62	38/23571 (0.2%)
2	C	0.45	2/2513 (0.1%)	0.82	12/3426 (0.4%)
2	D	0.69	6/2493 (0.2%)	0.72	7/3401 (0.2%)
All	All	0.40	24/37677 (0.1%)	0.60	73/51455 (0.1%)

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	3
1	B	0	5
2	D	0	2
All	All	0	10

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	330	CYS	C-O	-23.55	0.93	1.24
2	D	330	CYS	C-N	-5.83	1.25	1.33
1	B	751	HIS	ND1-CE1	5.61	1.38	1.32
1	B	737	HIS	ND1-CE1	5.45	1.38	1.32
1	B	830	HIS	ND1-CE1	5.42	1.38	1.32

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	682	CYS	N-CA-CB	14.97	132.13	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	330	CYS	N-CA-CB	14.64	134.69	110.39
1	B	1188	PHE	CB-CA-C	-13.90	89.17	110.02
1	B	1189	PRO	N-CA-C	-13.87	94.82	113.40
1	B	1767	THR	CA-CB-OG1	-11.30	92.64	109.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2333	ARG	Sidechain
1	A	2475	ASP	Mainchain
1	A	2547	ARG	Sidechain
1	B	1194	ARG	Sidechain
1	B	1767	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	15297	11475	11498	103	0
1	B	17039	14272	14390	220	0
2	C	2491	2088	2096	56	0
2	D	2472	2026	2034	55	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
4	C	1	0	0	0	0
All	All	37360	29861	30018	424	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 6.

The worst 5 of 424 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)
2:D:330:CYS:O	2:D:331:HIS:C	2.08	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:330:CYS:O	2:D:330:CYS:SG	2.35	0.84
1:B:2514:ARG:HG3	1:B:2519:MET:HE1	1.62	0.82
1:A:2366:ALA:HB1	1:A:2368:ILE:HD11	1.62	0.81
2:C:680:CYS:C	2:C:682:CYS:H	1.88	0.81

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	2451/2637 (93%)	2313 (94%)	136 (6%)	2 (0%)	48 79
1	B	2471/2637 (94%)	2327 (94%)	142 (6%)	2 (0%)	48 79
2	C	370/491 (75%)	341 (92%)	27 (7%)	2 (0%)	25 58
2	D	372/491 (76%)	336 (90%)	35 (9%)	1 (0%)	37 69
All	All	5664/6256 (90%)	5317 (94%)	340 (6%)	7 (0%)	50 79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
2	D	329	LEU
2	C	318	LYS
1	A	2328	PRO
2	C	629	GLY

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	1021/2358 (43%)	1013 (99%)	8 (1%)	79	84
1	B	1387/2358 (59%)	1376 (99%)	11 (1%)	79	84
2	C	207/417 (50%)	201 (97%)	6 (3%)	37	58
2	D	194/417 (46%)	190 (98%)	4 (2%)	48	66
All	All	2809/5550 (51%)	2780 (99%)	29 (1%)	71	80

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2327	LYS
2	C	630	CYS
1	B	2380	VAL
2	C	432	GLN
1	B	2377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2480	ASN
2	D	657	GLN
1	B	2517	HIS
2	D	424	GLN
2	C	584	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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	A1EIK	B	2701	-	31,35,35	0.80	1 (3%)	33,53,53	1.51	4 (12%)
3	A1EIK	A	2701	-	31,35,35	0.71	0	33,53,53	1.14	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	A1EIK	B	2701	-	-	2/10/44/44	0/7/6/6
3	A1EIK	A	2701	-	-	4/10/44/44	0/7/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	A1EIK	C15-N14	-2.25	1.40	1.44

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2701	A1EIK	O4-C3-C2	-5.84	94.99	111.48
3	A	2701	A1EIK	C21-C20-C11	-3.56	116.14	119.98
3	B	2701	A1EIK	C21-C20-C11	-3.25	116.47	119.98
3	B	2701	A1EIK	C8-N9-C10	-2.71	114.74	118.75
3	A	2701	A1EIK	C8-N9-C10	-2.48	115.09	118.75

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

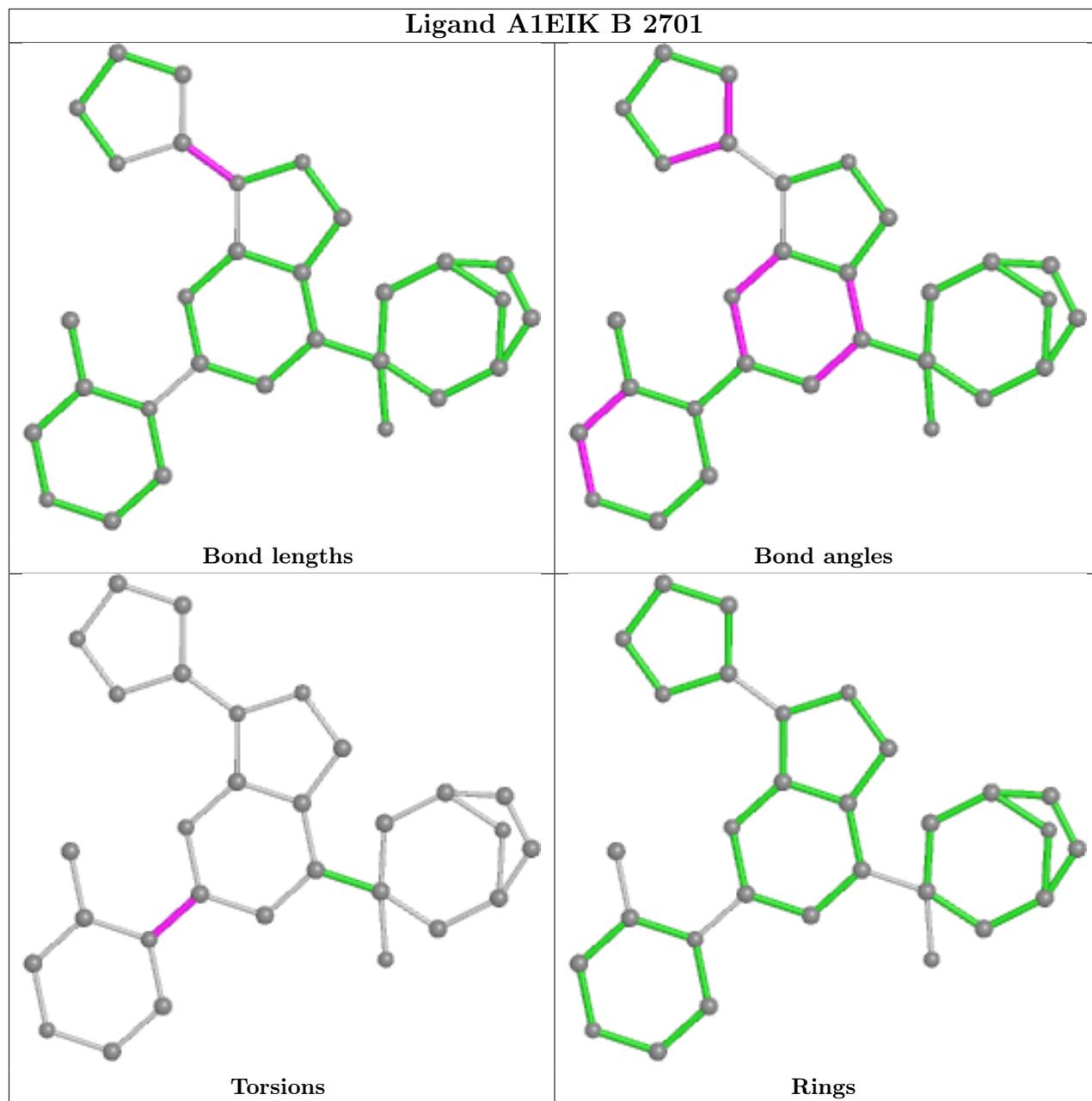
Mol	Chain	Res	Type	Atoms
3	A	2701	A1EIK	C21-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C6
3	A	2701	A1EIK	C21-C8-N7-C6
3	B	2701	A1EIK	C21-C8-N7-C2

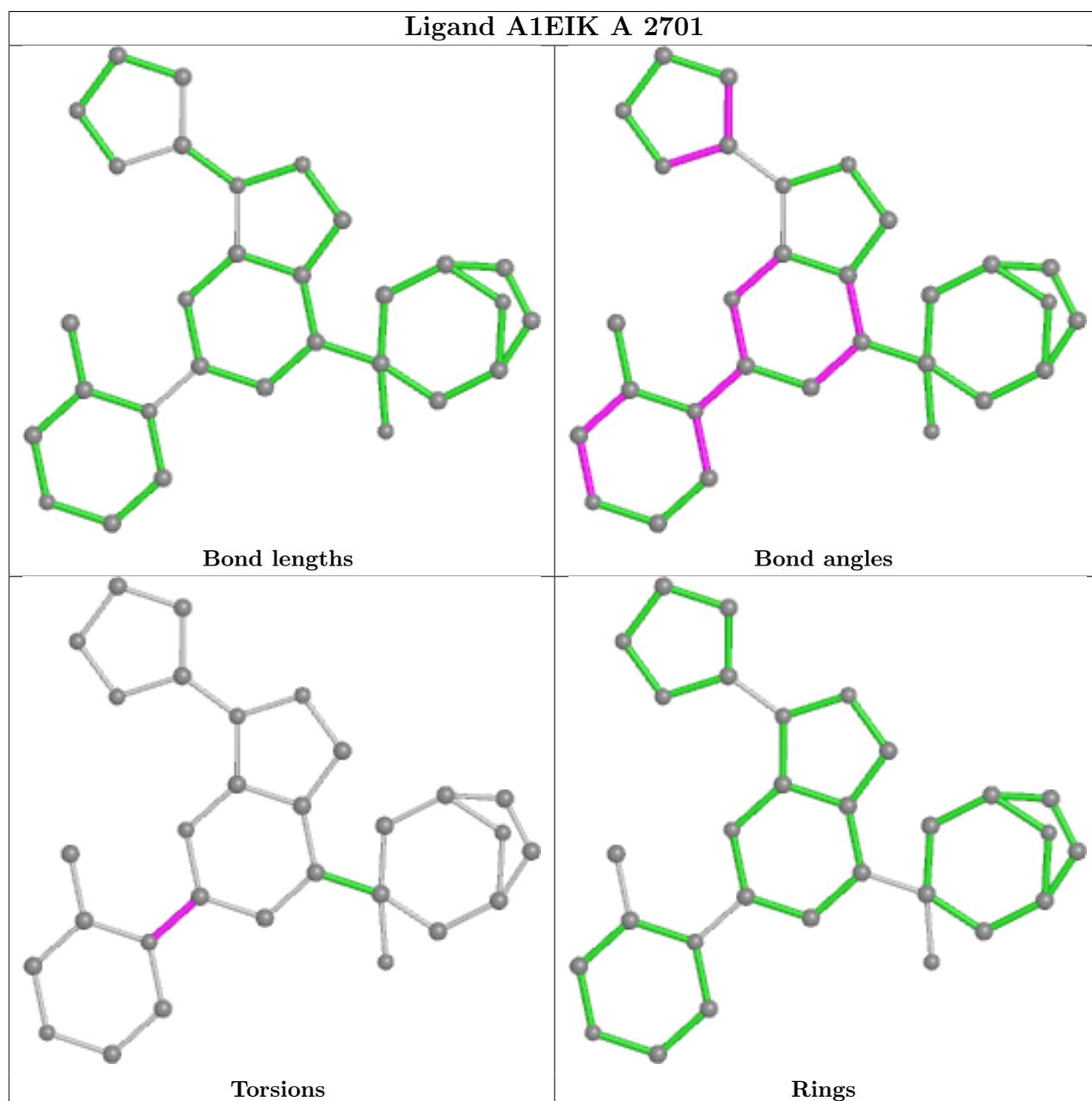
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.