wwPDB EM Validation Summary Report

May 25, 2025 – 12:21 AM JST

PDB ID	:	9L46 / pdb_00009l46
EMDB ID	:	EMD-62807
Title	:	ATR-ATRIP-bound with AMP-PNP
Authors	:	Wang, G.
Deposited on	:	2024-12-20
Resolution	:	6.29 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:

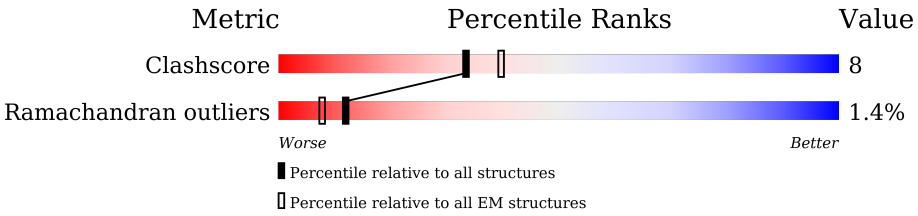
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.29 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

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	80% 9% 11%
1	B	2644	73% 9% • 17%
2	C	791	40% • 56%
2	D	791	33% • 66%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25683 atoms, of which 8 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.

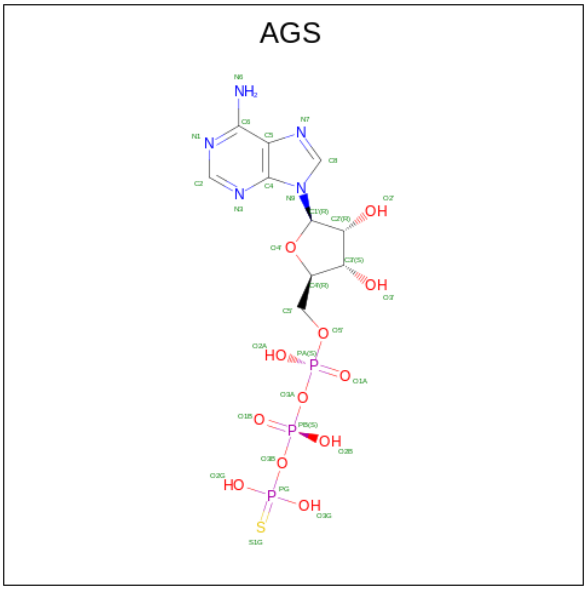
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2360	Total 11700	C 6979	N 2360	O 2361	0	0
1	B	2188	Total 10846	C 6469	N 2188	O 2189	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	270	Total 1339	C 799	N 270	O 270	0	0
2	C	349	Total 1728	C 1030	N 349	O 349	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



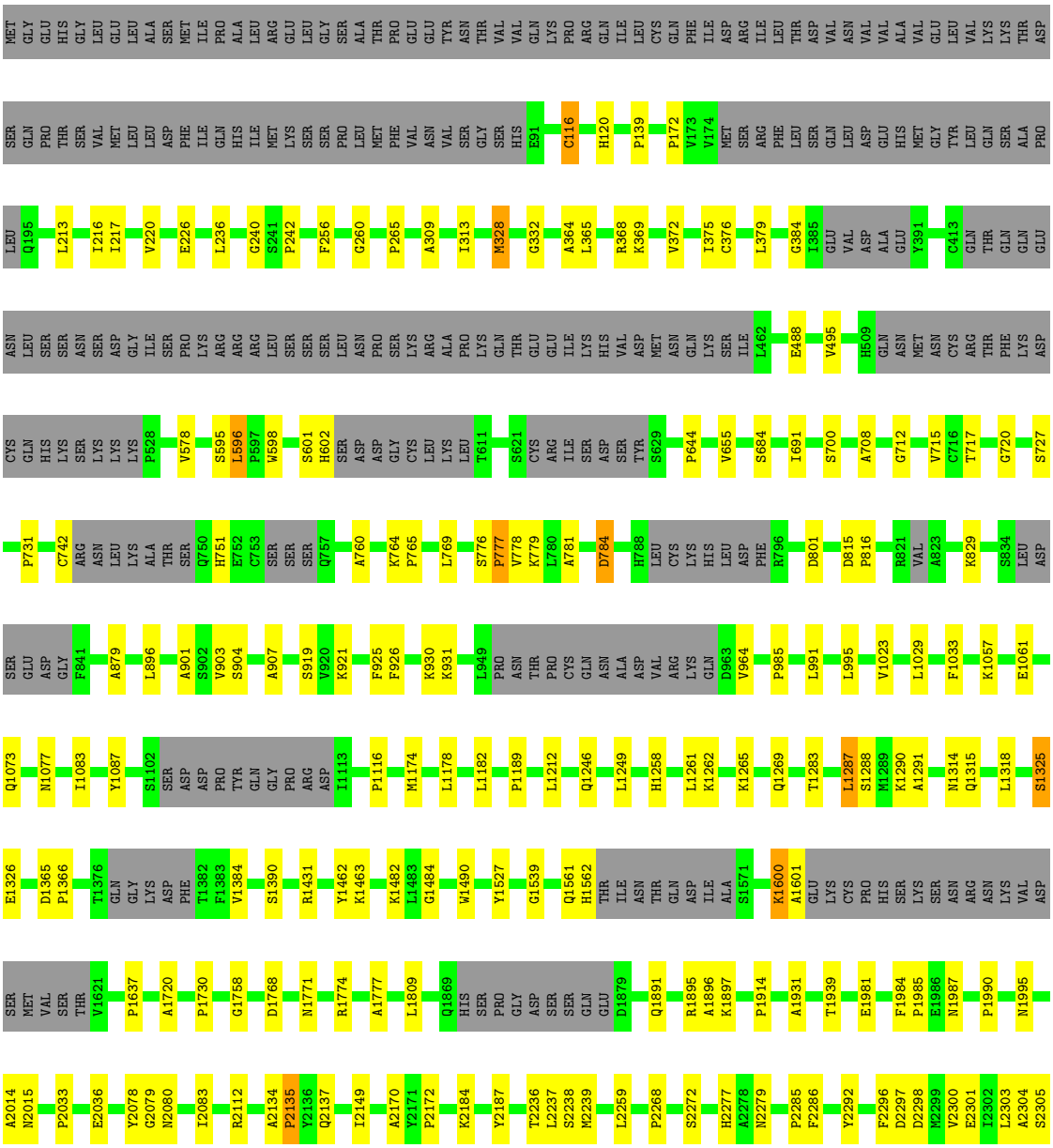
Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	H	N	O	P	S	0
			35	10	4	5	12	3	1	
3	B	1	Total	C	H	N	O	P	S	0
			35	10	4	5	12	3	1	

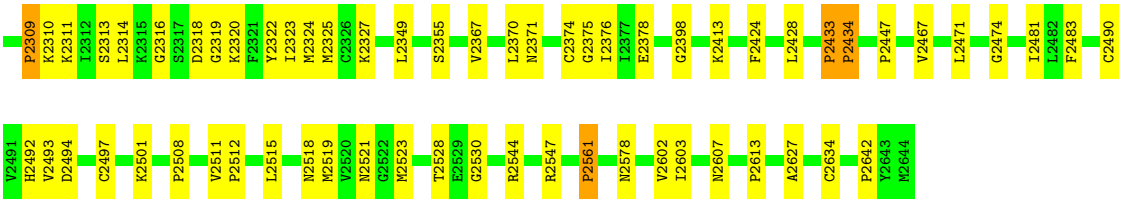
3 Residue-property plots (i)

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

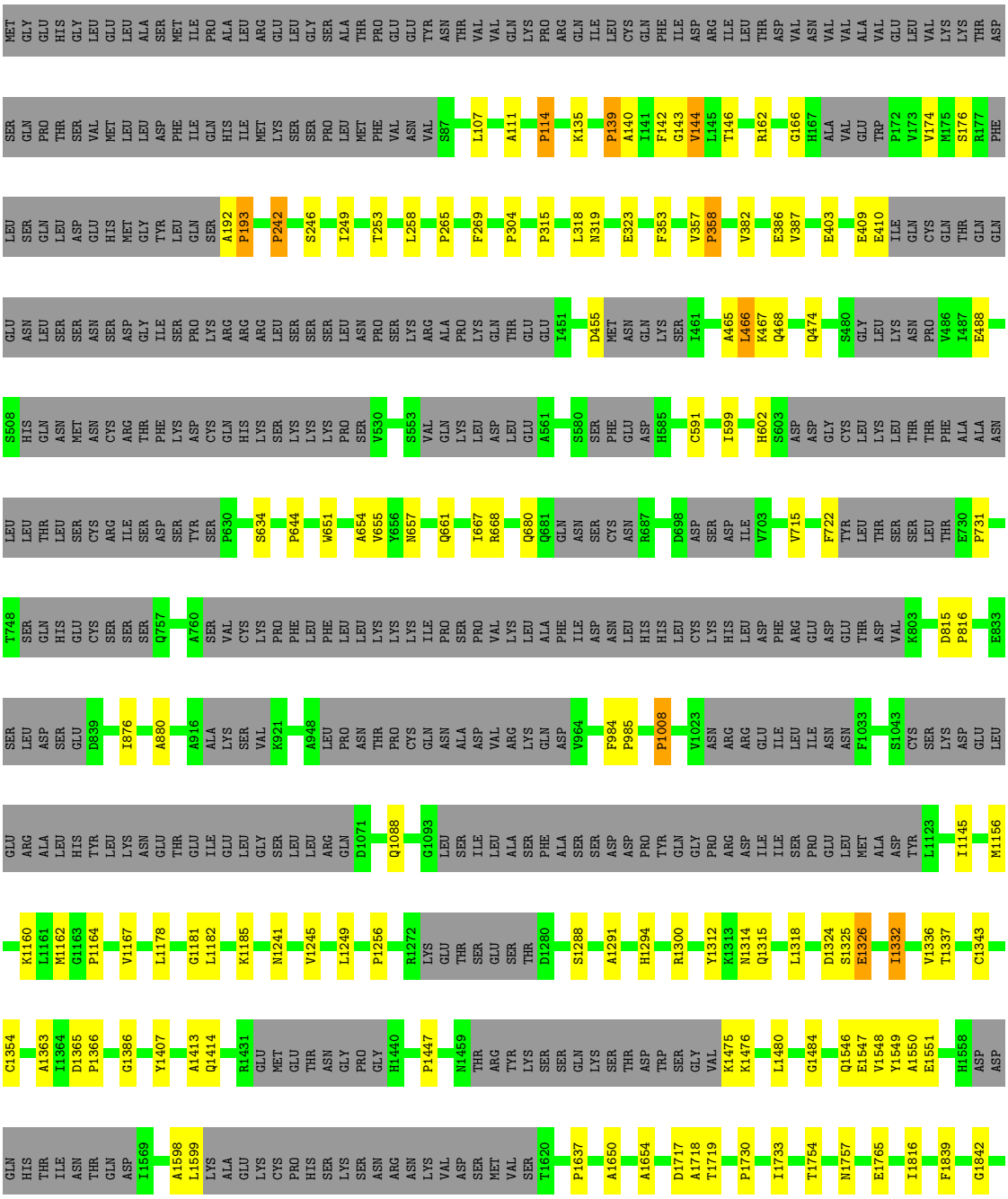
Chain A:

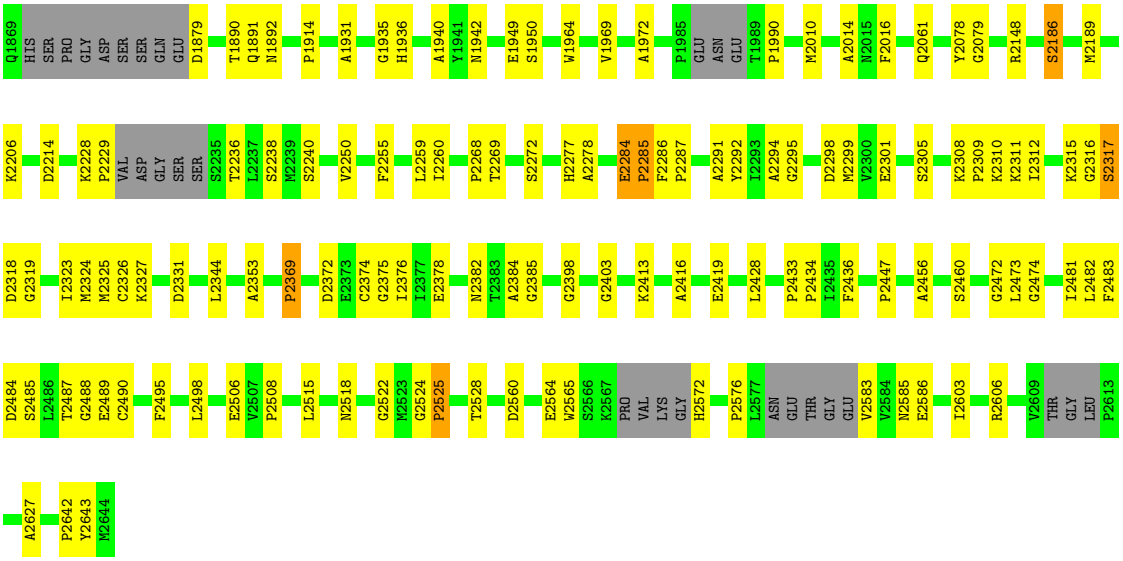




• Molecule 1: Serine/threonine-protein kinase ATR

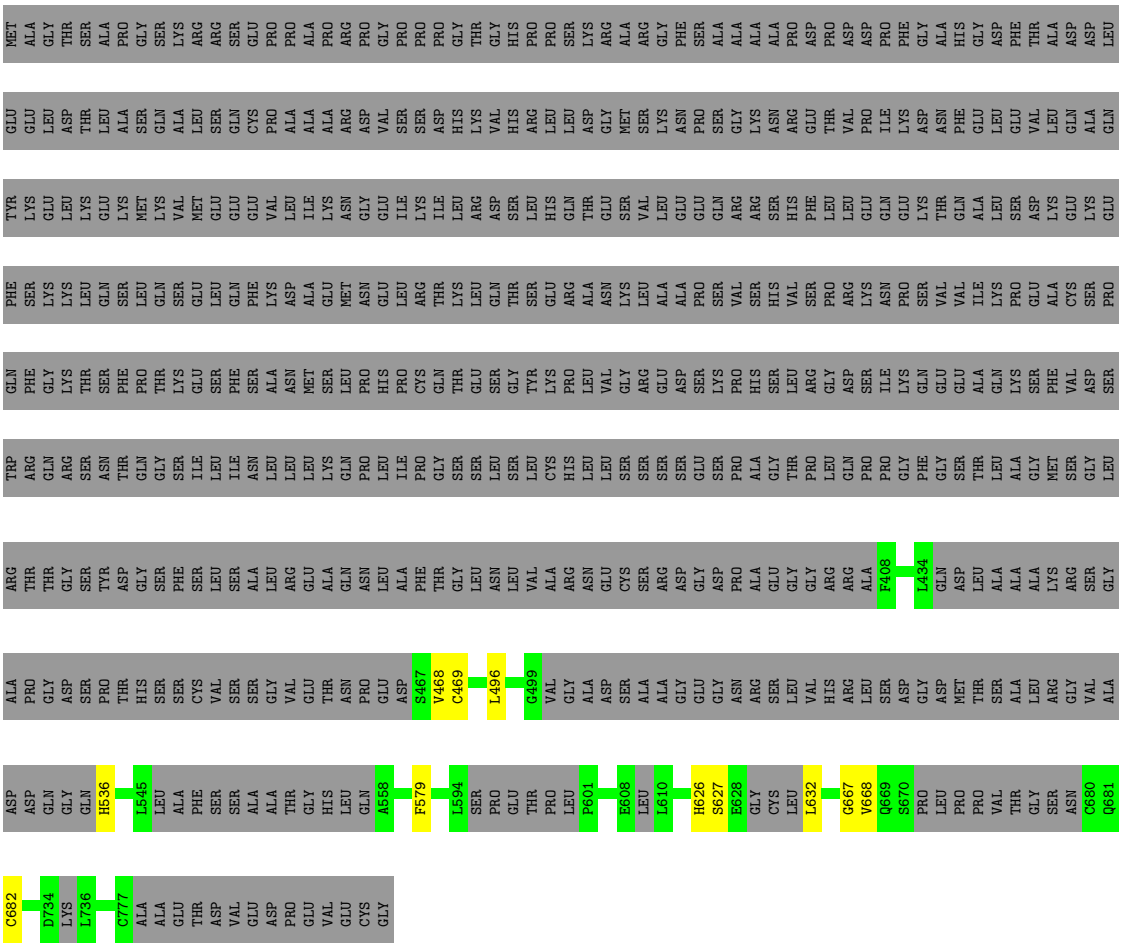
Chain B:





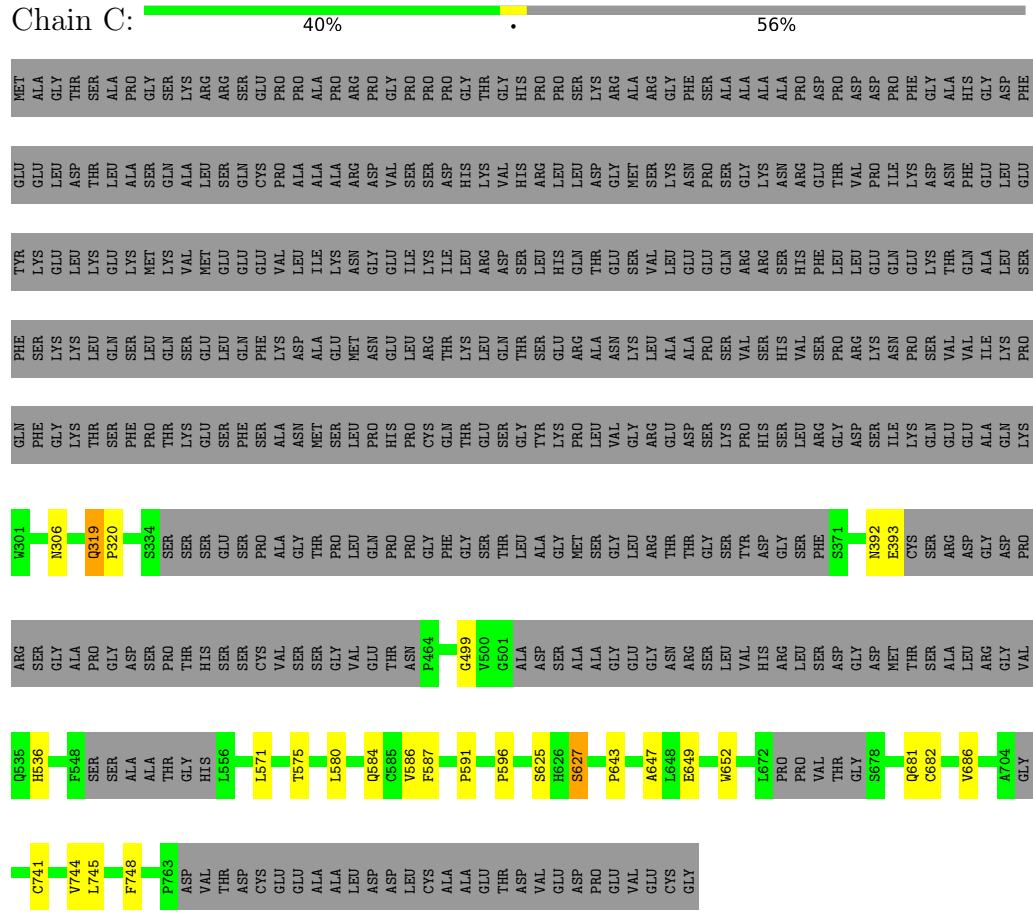
• Molecule 2: ATR-interacting protein

Chain D:



• Molecule 2: ATR-interacting protein

Chain C:


40%
56%
MET ALA GLY THR SER ALA PRO GLY SER LYS ARG ARG SER GLU PRO PRO ALA PRO ARG PRO GLY PRO PRO PRO GLY THR GLY HIS PRO PRO SER LYS ARG ALA ARG GLY PHE SER ALA ALA ALA PRO ASP PRO ASP ASP PRO PHE GLY ALA HIS GLY ASP PHE THR ALA ASP ASP LEU
GLU GLU LEU ASP THR LEU ALA SER GLN ALA LEU SER GLN CYS PRO ALA ALA ALA ARG ASP VAL SER SER ASP HIS LYS VAL HIS ARG LEU LEU ASP GLY MET SER LYS ASN PRO SER GLY LYS ASN ARG GLU THR VAL PRO ILE LYS ASP ASN PHE GLU GLU LEU GLU VAL LEU GLN ALA GLN
TYR LYS GLU LEU LYS GLU LYS MET LYS VAL MET GLU GLU GLU VAL LEU ILE LYS ASN GLY GLU ILE LYS ILE LEU ARG ASP SER LEU HIS GLN THR GLU SER VAL LEU GLU GLU GLN ARG ARG SER HIS PHE LEU LEU GLU GLN GLU LYS THR GLN ALA LEU SER ASP LYS GLU LYS GLU
PHE SER LYS LYS LEU GLN SER LEU GLN SER GLU LEU GLN PHE LYS ASP ALA GLU MET ASN GLU LEU ARG THR LYS LEU GLN THR SER GLU ARG ALA ASN LYS LEU ALA ALA PRO SER VAL SER HIS VAL SER PRO ARG LYS ASN PRO HIS SER ILE LYS GLN GLU GLU ALA GLN LYS SER PHE VAL ASP SER
GLN PHE GLY LYS THR SER PHE PRO THR LYS GLU SER PHE SER ALA ASN MET SER LEU PRO HIS PRO CYS GLN THR GLU SER GLY TYR LYS PRO LEU VAL GLY ARG GLU ASP SER LYS PRO HIS SER LEU ARG GLY ASP SER ILE LYS GLN GLU GLU ALA GLN LYS SER PHE VAL ASP SER
W301 N306 Q319 P320 S334 SER SER SER GLU SER PRO ALA GLY THR PRO LEU GLN PRO PRO GLY PHE GLY SER THR LEU ALA GLY MET SER GLY LEU ARG THR THR GLY SER TYR ASP GLY SER PHE S371 N392 E393 CYS SER ARG ASP GLY ASP PRO ALA GLU G403 K441
ARG SER GLY ALA PRO GLY ASP SER PRO THR HIS SER SER CYS VAL SER SER GLY VAL GLU GLU THR ASN P464 G499 V500 G501 ALA ASP SER ALA ALA GLY GLU GLY ASN ARG SER LEU VAL HIS ARG LEU SER ASP GLY ASP MET THR SER ALA LEU ARG GLY VAL ALA ASP ASP GLN G534
Q535 H536 F548 SER SER ALA ALA THR GLY HIS L556 L571 T575 L580 Q584 C585 V586 F587 P591 P596 S625 H626 S627 P643 A647 L648 E649 W652 L672 PRO PRO VAL THR GLY S678 Q681 C682 V686 A704 GLY GLY PRO P708 F737
C741 V744 L745 F748 P763 ASP VAL THR ASP CYS GLU GLU ALA ALA LEU ASP ASP LEU CYS ALA ALA GLU THR ASP VAL GLU ASP PRO GLU VAL GLU CYS GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6895	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: AGS

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	1.14	0/11682	1.63	42/16264 (0.3%)
1	B	1.14	0/10814	1.61	46/15030 (0.3%)
2	C	1.13	0/1720	1.56	7/2385 (0.3%)
2	D	1.15	0/1330	1.51	1/1841 (0.1%)
All	All	1.14	0/25546	1.61	96/35520 (0.3%)

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
2	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2433	PRO	N-CA-C	-11.02	97.25	110.70
1	A	784	ASP	CB-CA-C	-10.59	104.34	116.63
1	B	2285	PRO	N-CA-C	-10.34	99.15	113.53
1	B	1164	PRO	N-CA-C	-9.64	100.48	113.40
1	A	2433	PRO	N-CA-C	-9.17	99.51	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	777	PRO	Peptide
2	C	319	GLN	Peptide

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	11700	0	5197	131	0
1	B	10846	0	4822	153	0
2	C	1728	0	757	15	0
2	D	1339	0	575	9	0
3	A	31	4	12	1	0
3	B	31	4	12	2	0
All	All	25675	8	11375	300	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 8.

The worst 5 of 300 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:627:SER:O	2:D:682:CYS:CB	1.68	1.41
1:B:1315:GLN:CA	1:B:1879:ASP:HA	1.57	1.33
1:B:1315:GLN:HA	1:B:1879:ASP:CA	1.58	1.33
1:B:1475:LYS:O	1:B:1547:GLU:HA	1.23	1.26
1:B:2238:SER:HA	1:B:2299:MET:HA	1.22	1.19

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	2324/2644 (88%)	2189 (94%)	97 (4%)	38 (2%)	8 38
1	B	2124/2644 (80%)	2005 (94%)	89 (4%)	30 (1%)	9 40
2	C	333/791 (42%)	324 (97%)	9 (3%)	0	100 100
2	D	252/791 (32%)	244 (97%)	8 (3%)	0	100 100
All	All	5033/6870 (73%)	4762 (95%)	203 (4%)	68 (1%)	12 40

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	PRO
1	A	495	VAL
1	A	596	LEU
1	A	644	PRO
1	A	731	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	$\#\|Z\| > 2$
3	AGS	B	2701	-	26,33,33	0.82	1 (3%)	26,52,52	0.87	1 (3%)
3	AGS	A	2701	-	26,33,33	0.81	1 (3%)	26,52,52	0.76	1 (3%)

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	AGS	B	2701	-	-	5/17/38/38	0/3/3/3
3	AGS	A	2701	-	-	7/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	AGS	PG-S1G	2.14	1.95	1.90
3	A	2701	AGS	PG-S1G	2.06	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2701	AGS	C5-C6-N6	2.32	123.88	120.35
3	B	2701	AGS	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2701	AGS	PB-O3B-PG-O3G
3	A	2701	AGS	C5'-O5'-PA-O1A
3	B	2701	AGS	C3'-C4'-C5'-O5'
3	A	2701	AGS	O4'-C4'-C5'-O5'
3	B	2701	AGS	C4'-C5'-O5'-PA

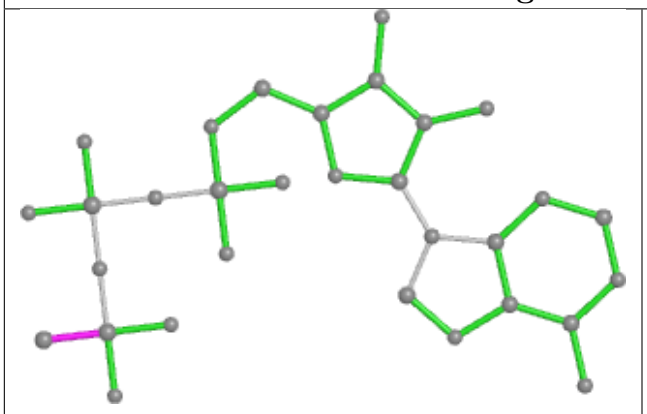
There are no ring outliers.

2 monomers are involved in 3 short contacts:

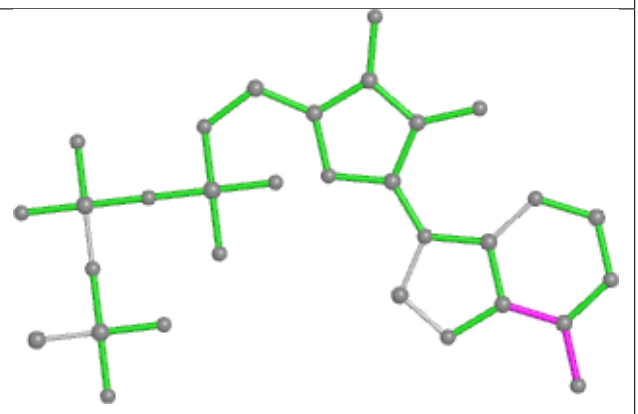
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2701	AGS	2	0
3	A	2701	AGS	1	0

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.

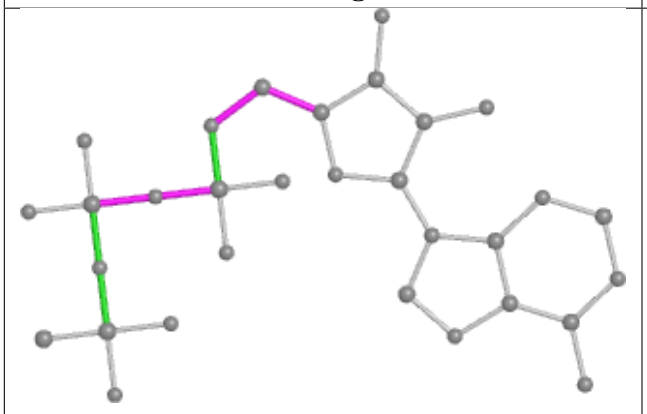
Ligand AGS B 2701



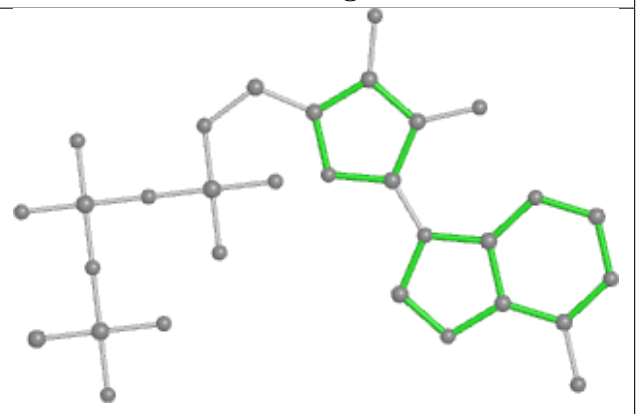
Bond lengths



Bond angles

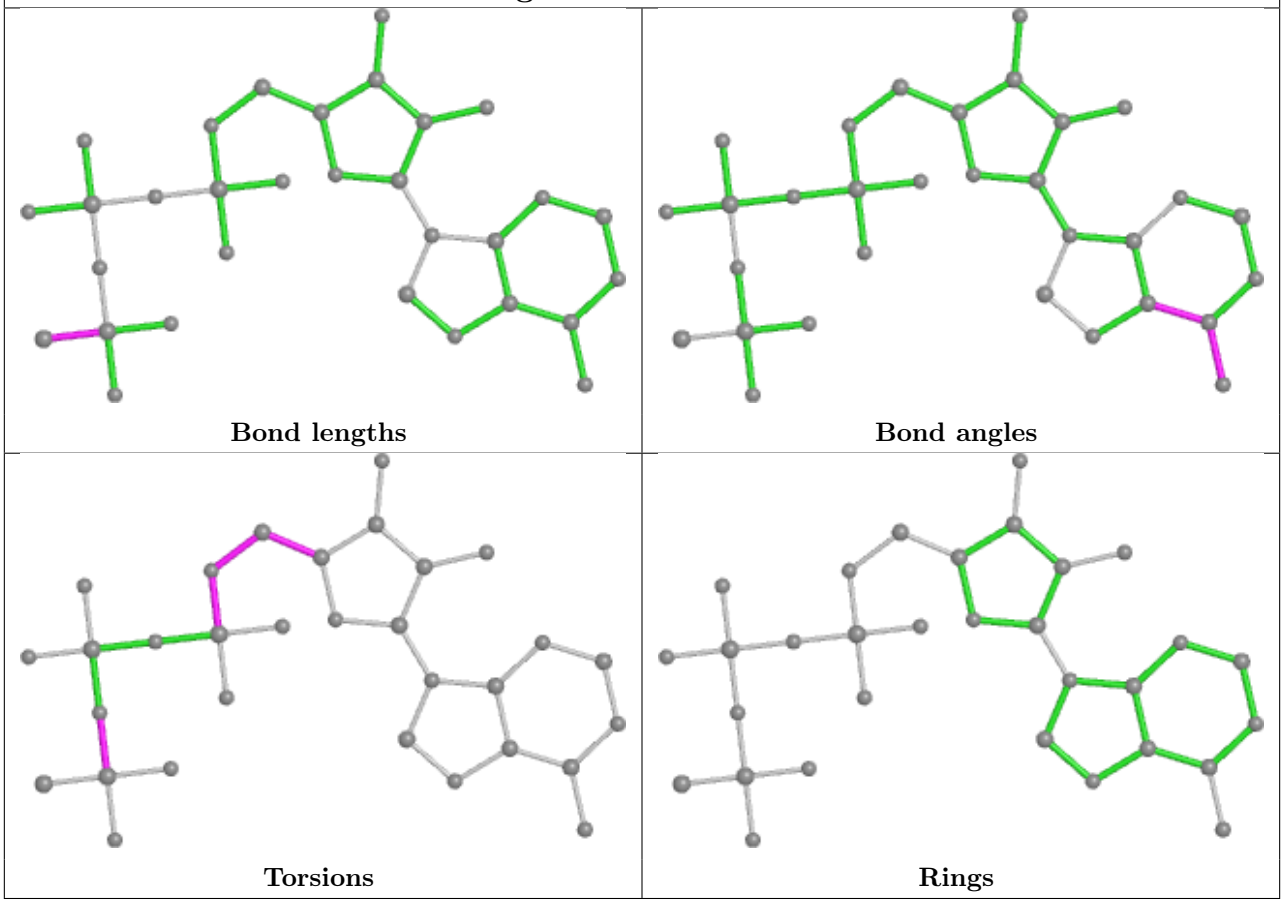


Torsions



Rings

Ligand AGS 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.