



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:40 PM UTC

PDB ID : 9FOY / pdb_00009foy
Title : Ternary complex of a Mycobacterium tuberculosis DNA gyrase core fusion with DNA and the inhibitor AMK32b
Authors : Kokot, M.; Hrast, M.; Feng, L.; Mitchenall, L.A.; Lawson, D.M.; Maxwell, A.; Minovski, N.; Anderluh, M.
Deposited on : 2024-06-12
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

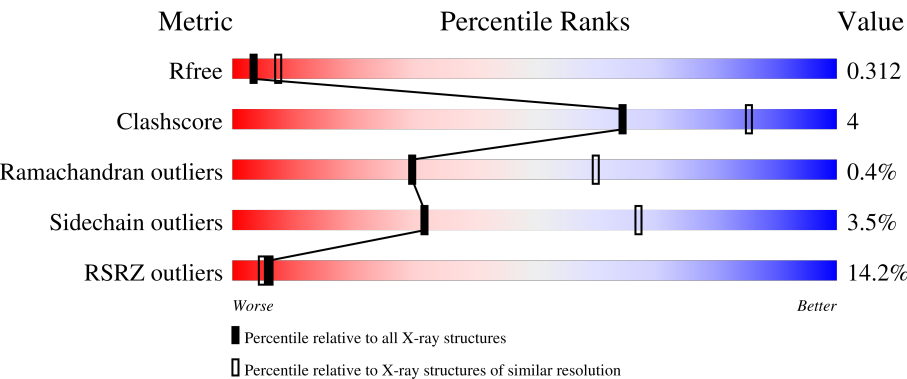
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	756	15% 84% 12% ..
1	B	756	12% 84% 12% ..
2	E	8	12% 88% 12%
2	G	8	25% 25% 62% 12%

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Mol	Chain	Length	Quality of chain
3	F	12	
3	H	12	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5718	3574	1041	1083	20			
1	B	730	Total	C	N	O	S	0	0	0
			5720	3573	1042	1085	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	SER	-	expression tag	UNP P9WG45
A	424	ASN	-	expression tag	UNP P9WG45
A	425	ALA	-	expression tag	UNP P9WG45
A	1501	ILE	-	expression tag	UNP P9WG47
A	1502	GLY	-	expression tag	UNP P9WG47
A	1503	SER	-	expression tag	UNP P9WG47
A	1504	GLY	-	expression tag	UNP P9WG47
B	423	SER	-	expression tag	UNP P9WG45
B	424	ASN	-	expression tag	UNP P9WG45
B	425	ALA	-	expression tag	UNP P9WG45
B	1501	ILE	-	expression tag	UNP P9WG47
B	1502	GLY	-	expression tag	UNP P9WG47
B	1503	SER	-	expression tag	UNP P9WG47
B	1504	GLY	-	expression tag	UNP P9WG47

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3').

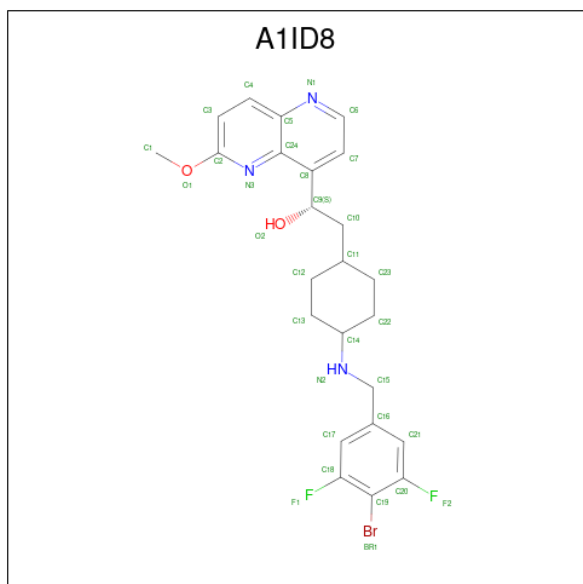
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
2	G	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP

*CP*T)-3').

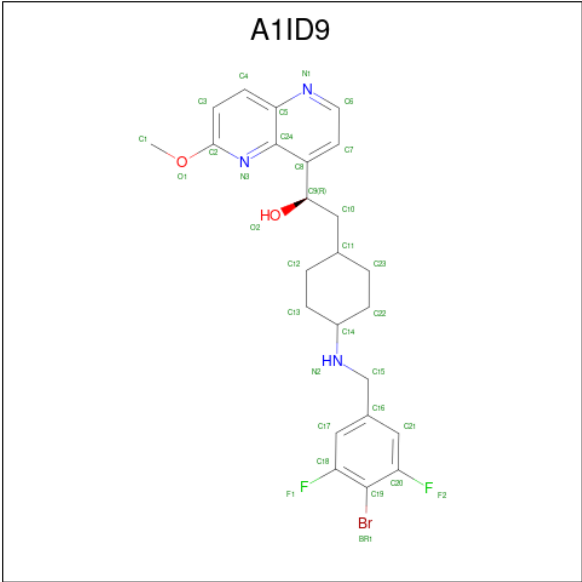
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			244	116	43	73	12			
3	H	12	Total	C	N	O	P	0	0	0
			244	116	43	73	12			

- Molecule 4 is (1 {S})-2-[4-[[4-bromanyl-3,5-bis(fluoranyl)phenyl]methylamino]cyclohexyl]-1-(6-methoxy-1,5-naphthyridin-4-yl)ethanol (CCD ID: A1ID8) (formula: C₂₄H₂₆BrF₂N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	H	1	Total	Br	C	F	N	O	0	0
			32	1	24	2	3	2		

- Molecule 5 is (1 {R})-2-[4-[[4-bromanyl-3,5-bis(fluoranyl)phenyl]methylamino]cyclohexyl]-1-(6-methoxy-1,5-naphthyridin-4-yl)ethanol (CCD ID: A1ID9) (formula: C₂₄H₂₆BrF₂N₃O₂) (labeled as "Ligand of Interest" by depositor).

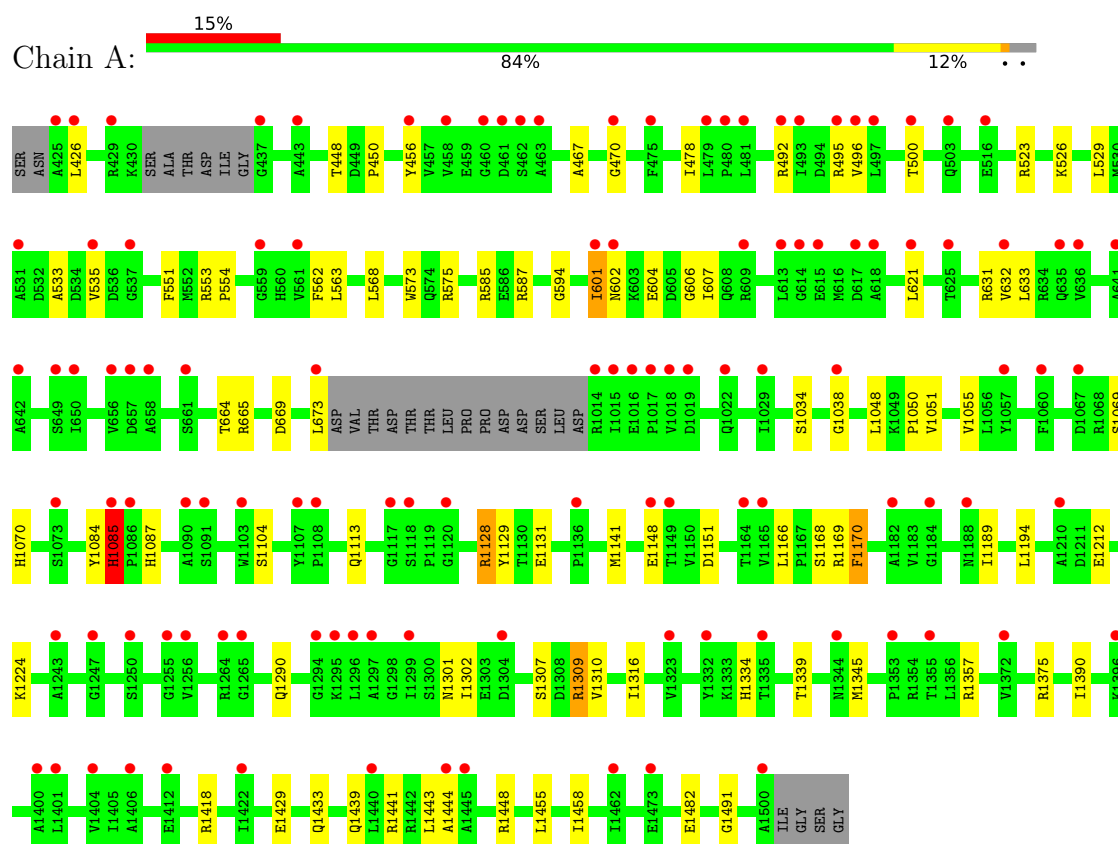


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	Br	C	F	N	O	0	0
			32	1	24	2	3	2		

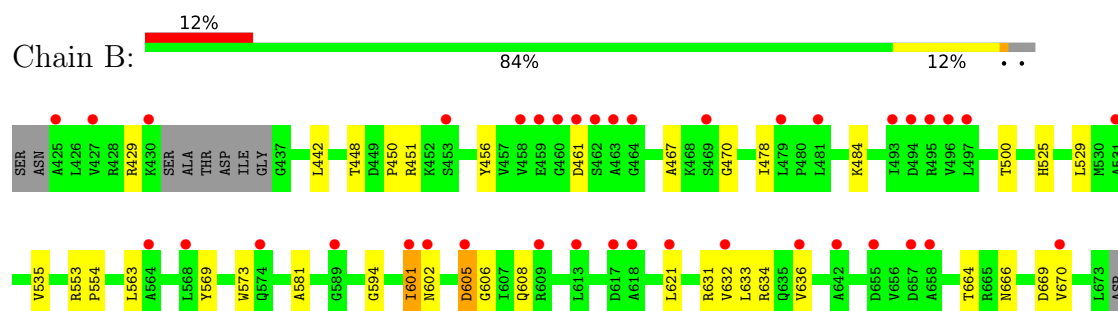
3 Residue-property plots [i](#)

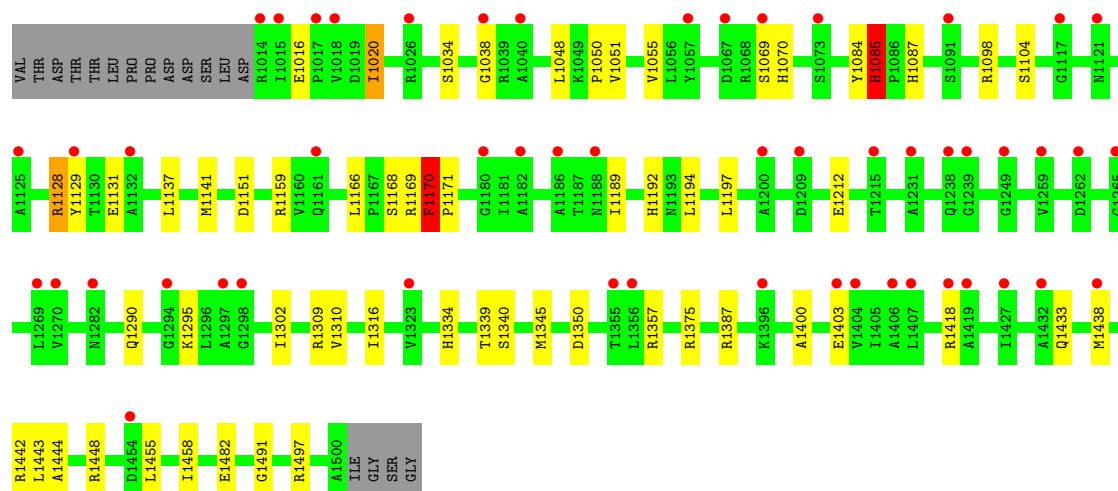
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA gyrase subunit B,DNA gyrase subunit A

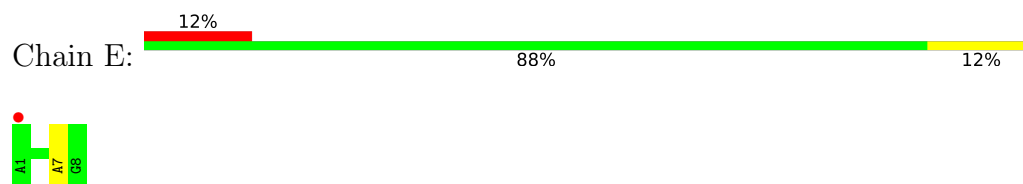


- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A





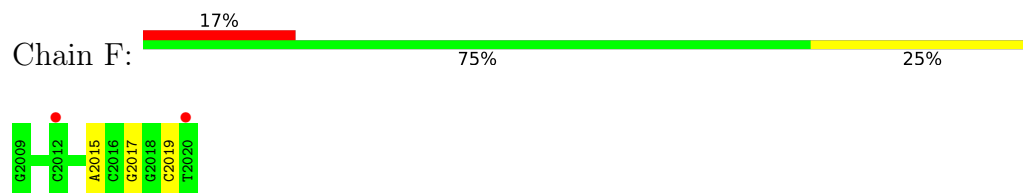
- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3')



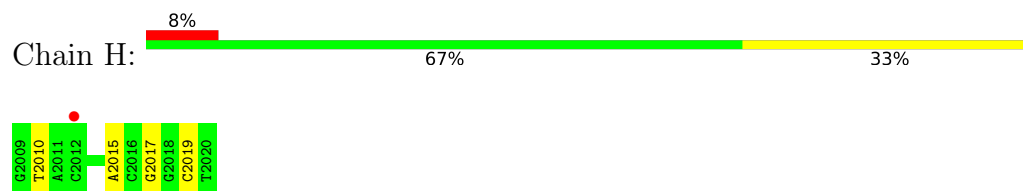
- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3')



- Molecule 3: DNA (5'-D(P*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



- Molecule 3: DNA (5'-D(P*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.04Å 131.70Å 96.28Å 90.00° 97.23° 90.00°	Depositor
Resolution (Å)	69.23 – 2.80 69.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.23-2.80) 100.0 (69.23-2.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.279 , 0.304 0.284 , 0.312	Depositor DCC
R_{free} test set	2542 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	12316	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: A1ID8, A1ID9

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	0.91	0/5805	1.34	3/7848 (0.0%)
1	B	0.91	0/5807	1.35	3/7849 (0.0%)
2	E	0.67	0/183	1.01	0/281
2	G	0.65	0/183	1.05	2/281 (0.7%)
3	F	0.70	0/272	1.10	3/417 (0.7%)
3	H	0.70	0/272	1.09	3/417 (0.7%)
All	All	0.89	0/12522	1.33	14/17093 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1170	PHE	CB-CA-C	6.86	118.16	108.76
1	A	1170	PHE	CB-CA-C	6.80	118.08	108.76
3	H	2015	DA	P-O3'-C3'	-6.06	111.11	120.20
3	F	2015	DA	P-O3'-C3'	-6.01	111.18	120.20
1	B	1087	HIS	CA-C-N	5.94	125.74	120.10

There are no chirality outliers.

There are no planarity outliers.

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	5718	0	5744	45	0
1	B	5720	0	5741	50	0
2	E	163	0	91	2	0
2	G	163	0	91	4	0
3	F	244	0	136	0	0
3	H	244	0	136	1	0
4	H	32	0	0	0	0
5	H	32	0	0	0	0
All	All	12316	0	11939	94	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 4.

The worst 5 of 94 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:1085:HIS:HE2	2:E:7:DA:P	2.15	0.70
1:B:1085:HIS:HE2	2:G:7:DA:P	2.18	0.67
1:B:429:ARG:NH1	1:B:442:LEU:O	2.27	0.66
1:A:1169:ARG:NH2	1:A:1482:GLU:OE2	2.28	0.66
1:B:1169:ARG:NH2	1:B:1482:GLU:OE2	2.29	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	724/756 (96%)	698 (96%)	23 (3%)	3 (0%)	30 60
1	B	724/756 (96%)	697 (96%)	24 (3%)	3 (0%)	30 60
All	All	1448/1512 (96%)	1395 (96%)	47 (3%)	6 (0%)	30 60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	GLU
1	B	605	ASP
1	A	1085	HIS
1	B	1085	HIS
1	A	601	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/632 (96%)	582 (96%)	22 (4%)	31	66
1	B	604/632 (96%)	584 (97%)	20 (3%)	33	69
All	All	1208/1264 (96%)	1166 (96%)	42 (4%)	32	67

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1020	ILE
1	B	1310	VAL
1	B	1069	SER
1	B	1128	ARG
1	B	1339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	574	GLN
1	B	602	ASN
1	B	1490	HIS
1	B	1290	GLN
1	B	1334	HIS

5.3.3 RNA ⓘ

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	$\# Z > 2$
4	A1ID8	H	2101	5	35,35,35	0.43	0	43,49,49	0.52	0
5	A1ID9	H	2102	4	35,35,35	0.41	0	43,49,49	0.52	0

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
4	A1ID8	H	2101	5	-	5/15/25/25	0/4/4/4
5	A1ID9	H	2102	4	-	8/15/25/25	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2101	A1ID8	C7-C8-C9-C10
4	H	2101	A1ID8	C24-C8-C9-C10

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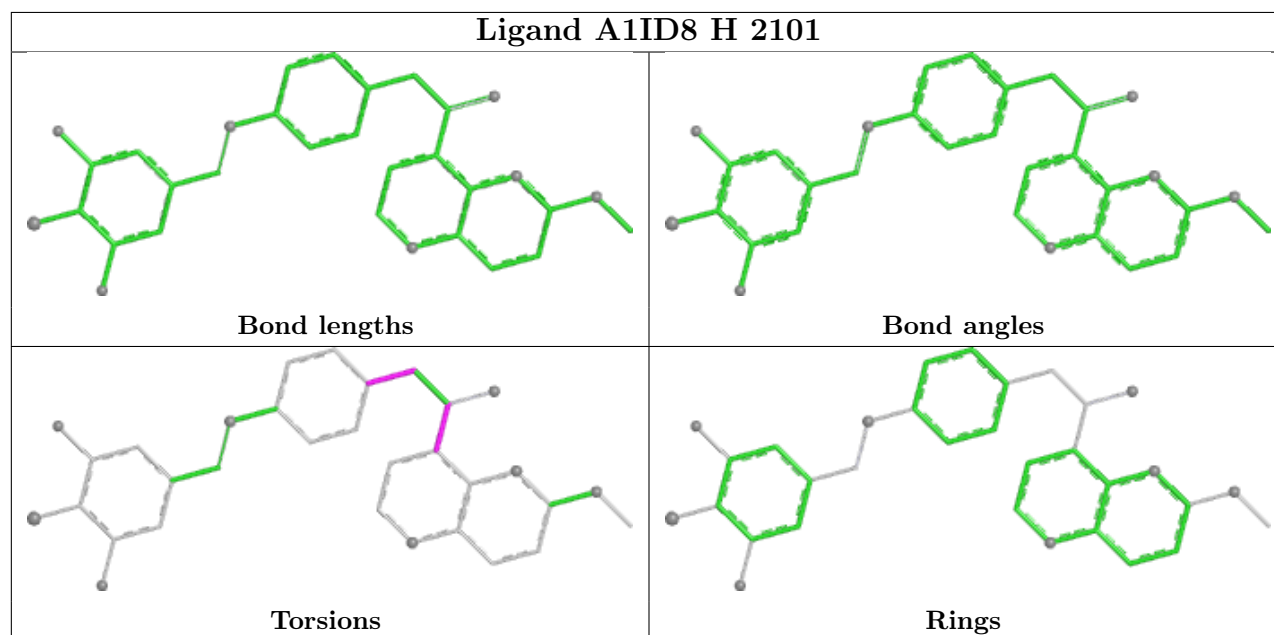
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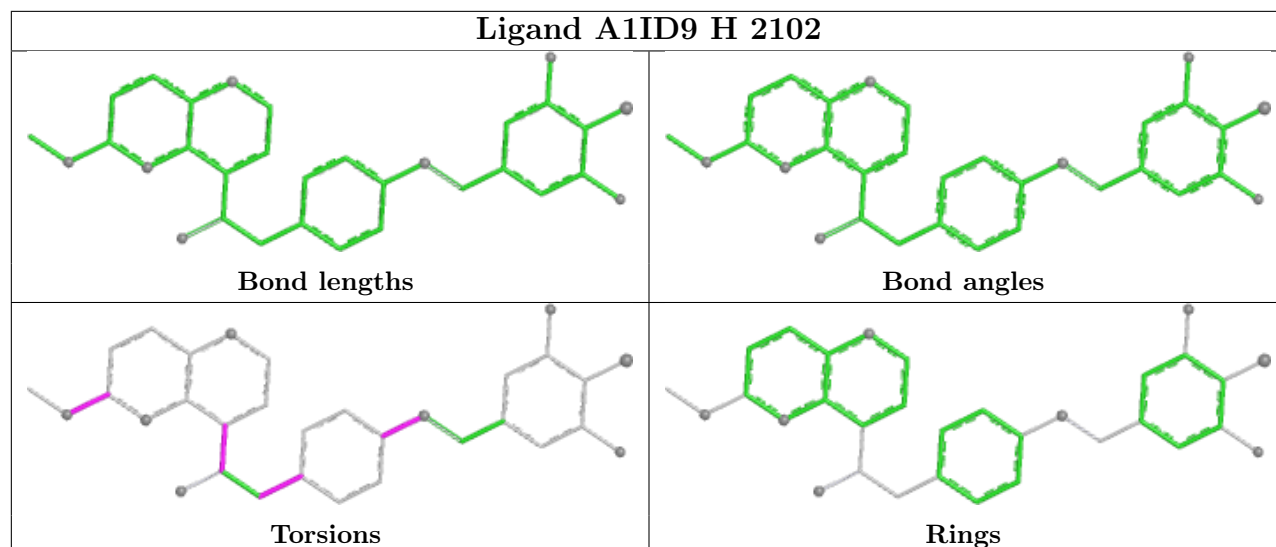
Mol	Chain	Res	Type	Atoms
5	H	2102	A1ID9	C7-C8-C9-C10
5	H	2102	A1ID9	C24-C8-C9-C10
5	H	2102	A1ID9	C13-C14-N2-C15

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	730/756 (96%)	1.23	116 (15%) 5 4	32, 44, 59, 66	0
1	B	730/756 (96%)	1.14	91 (12%) 8 6	32, 41, 57, 68	0
2	E	8/8 (100%)	1.14	1 (12%) 8 6	27, 36, 65, 72	0
2	G	8/8 (100%)	0.91	2 (25%) 2 1	27, 35, 54, 57	0
3	F	12/12 (100%)	1.12	2 (16%) 4 3	34, 39, 52, 59	0
3	H	12/12 (100%)	1.13	1 (8%) 17 12	35, 38, 55, 60	0
All	All	1500/1552 (96%)	1.18	213 (14%) 6 5	27, 42, 58, 72	0

The worst 5 of 213 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	613	LEU	5.2
1	B	1121	ASN	4.4
1	B	469	SER	4.2
1	B	458	VAL	4.0
1	A	1255	GLY	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

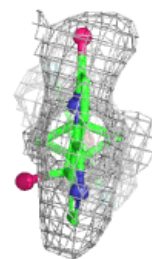
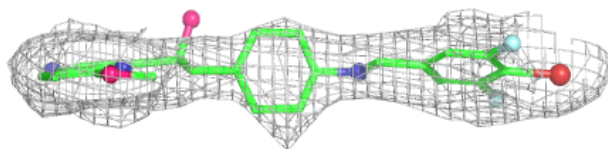
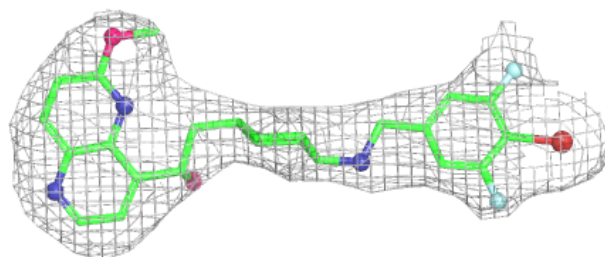
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1ID8	H	2101	32/32	0.92	0.14	38,38,39,39	32
5	A1ID9	H	2102	32/32	0.93	0.13	37,37,38,38	32

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

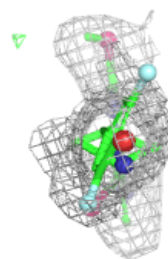
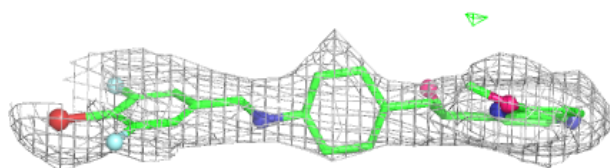
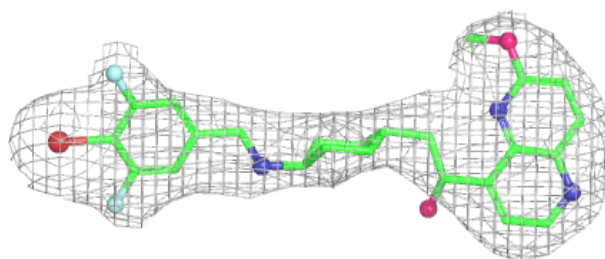
Electron density around A1ID8 H 2101:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1ID9 H 2102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.