



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 05:26 PM BST

PDB ID : 3U17
Title : Structure of BasE N-terminal domain from *Acinetobacter baumannii* bound to 6-(p-benzoyl)phenyl-1-(pyridin-4-ylmethyl)-1H-pyrazolo[3,4-b]pyridine-4-carboxylic acid
Authors : Gulick, A.M.; Drake, E.J.; Aldrich, C.C.; Neres, J.
Deposited on : 2011-09-29
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

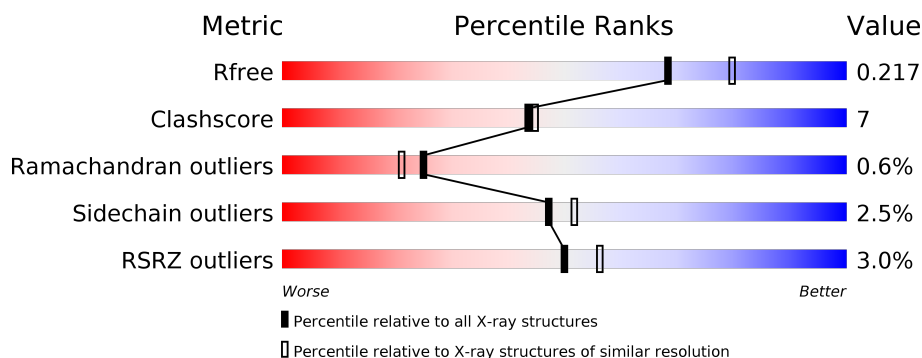
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	544	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>10%</div> <div>20%</div> </div> </div>
1	B	544	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>20%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7241 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.

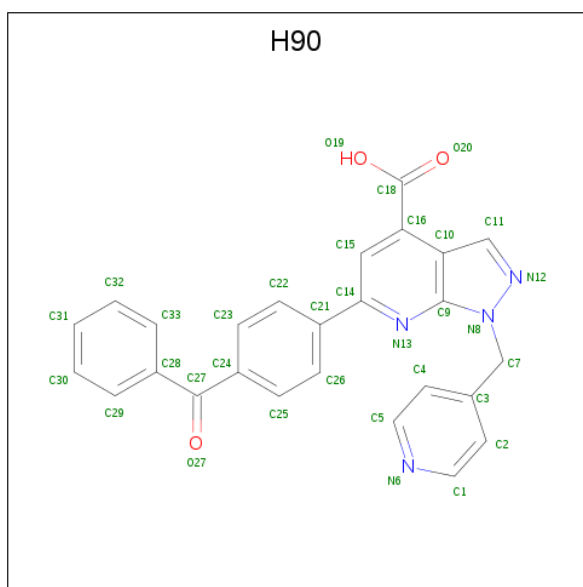
- Molecule 1 is a protein called Peptide arylation enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	2	0
			3382	2152	581	634	15			
1	B	436	Total	C	N	O	S	0	1	0
			3389	2160	574	640	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B2HVG8
A	0	HIS	-	expression tag	UNP B2HVG8
A	45	LEU	PRO	SEE REMARK 999	UNP B2HVG8
A	68	THR	SER	SEE REMARK 999	UNP B2HVG8
A	149	ASP	GLU	SEE REMARK 999	UNP B2HVG8
A	180	PHE	LEU	SEE REMARK 999	UNP B2HVG8
A	226	GLY	ASP	SEE REMARK 999	UNP B2HVG8
A	329	LEU	ILE	SEE REMARK 999	UNP B2HVG8
A	378	ARG	LYS	SEE REMARK 999	UNP B2HVG8
B	-1	GLY	-	expression tag	UNP B2HVG8
B	0	HIS	-	expression tag	UNP B2HVG8
B	45	LEU	PRO	SEE REMARK 999	UNP B2HVG8
B	68	THR	SER	SEE REMARK 999	UNP B2HVG8
B	149	ASP	GLU	SEE REMARK 999	UNP B2HVG8
B	180	PHE	LEU	SEE REMARK 999	UNP B2HVG8
B	226	GLY	ASP	SEE REMARK 999	UNP B2HVG8
B	329	LEU	ILE	SEE REMARK 999	UNP B2HVG8
B	378	ARG	LYS	SEE REMARK 999	UNP B2HVG8

- Molecule 2 is 6-(4-benzoylphenyl)-1-(pyridin-4-ylmethyl)-1H-pyrazolo[3,4-b]pyridine-4-carboxylic acid (three-letter code: H90) (formula: C₂₆H₁₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	26	4	3		
2	B	1	Total	C	N	O	0	0
			33	26	4	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

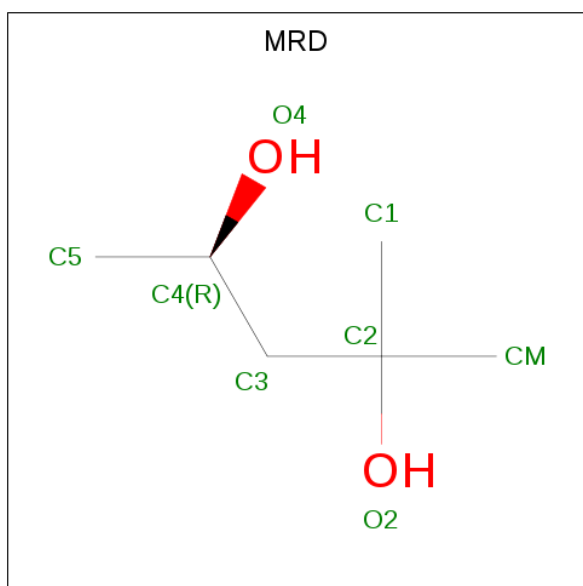
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total 184	O 184	0	0
6	B	197	Total 197	O 197	0	0

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.

[illegible]

Chain B:

Sequence logo for Chain B, showing amino acid conservation across 300 positions. The y-axis represents information content in bits (0.00 to 0.04). The x-axis shows positions 1 to 300. A color scale at the top indicates conservation levels: 29% (red), 67% (green), 12% (yellow), and 20% (grey). Amino acids are labeled above the bars, with some highlighted in red or orange. Red dots above the bars indicate specific positions of interest.

Position	Amino Acid
1	THR
2	SER
3	SER
4	THR
5	THR
6	SER
7	LYS
8	SER
9	CYS
10	ALA
11	PHE
12	ILE
13	VAL
14	SER
15	SER
16	ARG
17	ASN
18	PRO
19	GLU
20	LEU
21	LYS
22	ALA
23	VAL
24	VAL
25	LEU
26	ARG
27	ARG
28	HIS
29	LEU
30	ILE
31	ASN
32	GLU
33	LEU
34	ILE
35	ALA
36	GLN
37	LYS
38	LEU
39	PRO
40	GLU
41	ASP
42	ILE
43	GLU
44	LYS
45	LEU
46	ILE
47	GLU
48	SER
49	LEU
50	PRO
51	LEU
52	THR
53	ALA
54	VAL
55	GLY
56	LYS
57	ASP
58	VAL
59	LYS
60	GLN
61	ASP
62	GLU
63	ILE
64	PHE
65	GLY
66	ASN
67	GLU
68	THR
69	SER
70	THR
71	THR
72	THR
73	SER
74	THR
75	THR
76	THR
77	THR
78	THR
79	THR
80	THR
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210	THR
211	THR
212	THR
213	THR
214	THR
215	THR
216	THR
217	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.37Å 144.23Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 45.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.1 (40.00-2.10) 90.1 (45.75-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2), REFMAC (Diff. Fourier)	Depositor
R, R_{free}	0.189 , 0.221 0.185 , 0.217	Depositor DCC
R_{free} test set	3724 reflections (4.99%)	wwPDB-VI
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7241	wwPDB-VI
Average B, all atoms (Å ²)	41.0	wwPDB-VI

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H90, MRD, CA, MPD

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	0.37	0/3461	0.52	0/4711
1	B	0.37	0/3471	0.51	0/4728
All	All	0.37	0/6932	0.51	0/9439

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3382	0	3302	45	0
1	B	3389	0	3292	44	0
2	A	33	0	17	3	0
2	B	33	0	17	2	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	8	0	14	1	0
5	B	8	0	14	0	0
6	A	184	0	0	3	0
6	B	197	0	0	1	0
All	All	7241	0	6656	91	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 7.

The worst 5 of 91 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:305[A]:GLN:HE22	1:A:330:ASN:HD22	1.11	0.94
1:A:401:GLN:HG2	6:A:585:HOH:O	1.72	0.88
1:A:106:LEU:HD11	1:A:196:LEU:HD21	1.63	0.81
1:B:269:LEU:H	1:B:269:LEU:HD12	1.48	0.79
1:A:228:ASN:HD22	1:A:230:ASN:H	1.30	0.78

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	431/544 (79%)	420 (97%)	10 (2%)	1 (0%)	47	49
1	B	435/544 (80%)	422 (97%)	9 (2%)	4 (1%)	17	12
All	All	866/1088 (80%)	842 (97%)	19 (2%)	5 (1%)	25	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	SER
1	B	315	ALA
1	B	269	LEU
1	B	270	ASN
1	A	203	THR

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	366/472 (78%)	357 (98%)	9 (2%)	47	52
1	B	366/472 (78%)	357 (98%)	9 (2%)	47	52
All	All	732/944 (78%)	714 (98%)	18 (2%)	47	52

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	PHE
1	B	44	SER
1	B	295	GLU
1	A	223	GLU
1	A	228	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	B	17	GLN
1	B	142	GLN
1	A	270	ASN
1	B	195	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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$
4	MPD	A	548	-	7,7,7	0.35	0	9,10,10	0.59	0
5	MRD	B	547	-	7,7,7	0.33	0	9,10,10	0.54	0
2	H90	A	543	-	33,37,37	1.03	1 (3%)	41,52,52	1.84	6 (14%)
2	H90	B	543	-	33,37,37	0.97	2 (6%)	41,52,52	1.82	8 (19%)

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	MPD	A	548	-	-	0/5/5/5	-
5	MRD	B	547	-	-	2/5/5/5	-
2	H90	A	543	-	-	0/16/20/20	0/5/5/5
2	H90	B	543	-	-	0/16/20/20	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	543	H90	C16-C18	3.92	1.51	1.47
2	B	543	H90	C16-C18	3.26	1.50	1.47
2	B	543	H90	C10-C9	-2.14	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	543	H90	C11-C10-C9	6.14	110.88	105.20
2	B	543	H90	C11-C10-C9	5.81	110.57	105.20
2	A	543	H90	C3-C7-N8	-5.81	103.98	112.48
2	B	543	H90	C3-C7-N8	-4.65	105.67	112.48
2	B	543	H90	C16-C15-C14	-3.45	119.32	121.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

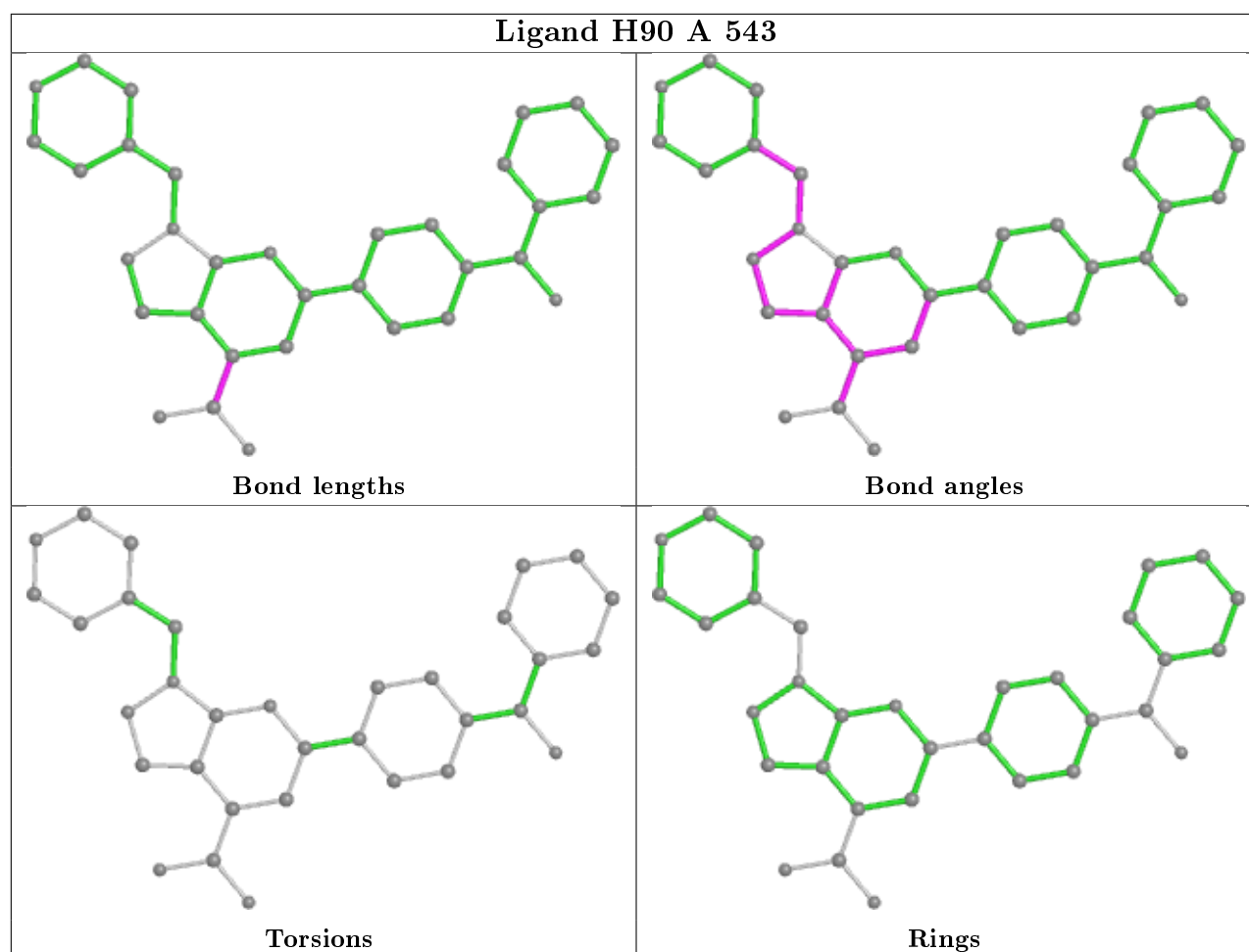
Mol	Chain	Res	Type	Atoms
5	B	547	MRD	C2-C3-C4-C5
5	B	547	MRD	C2-C3-C4-O4

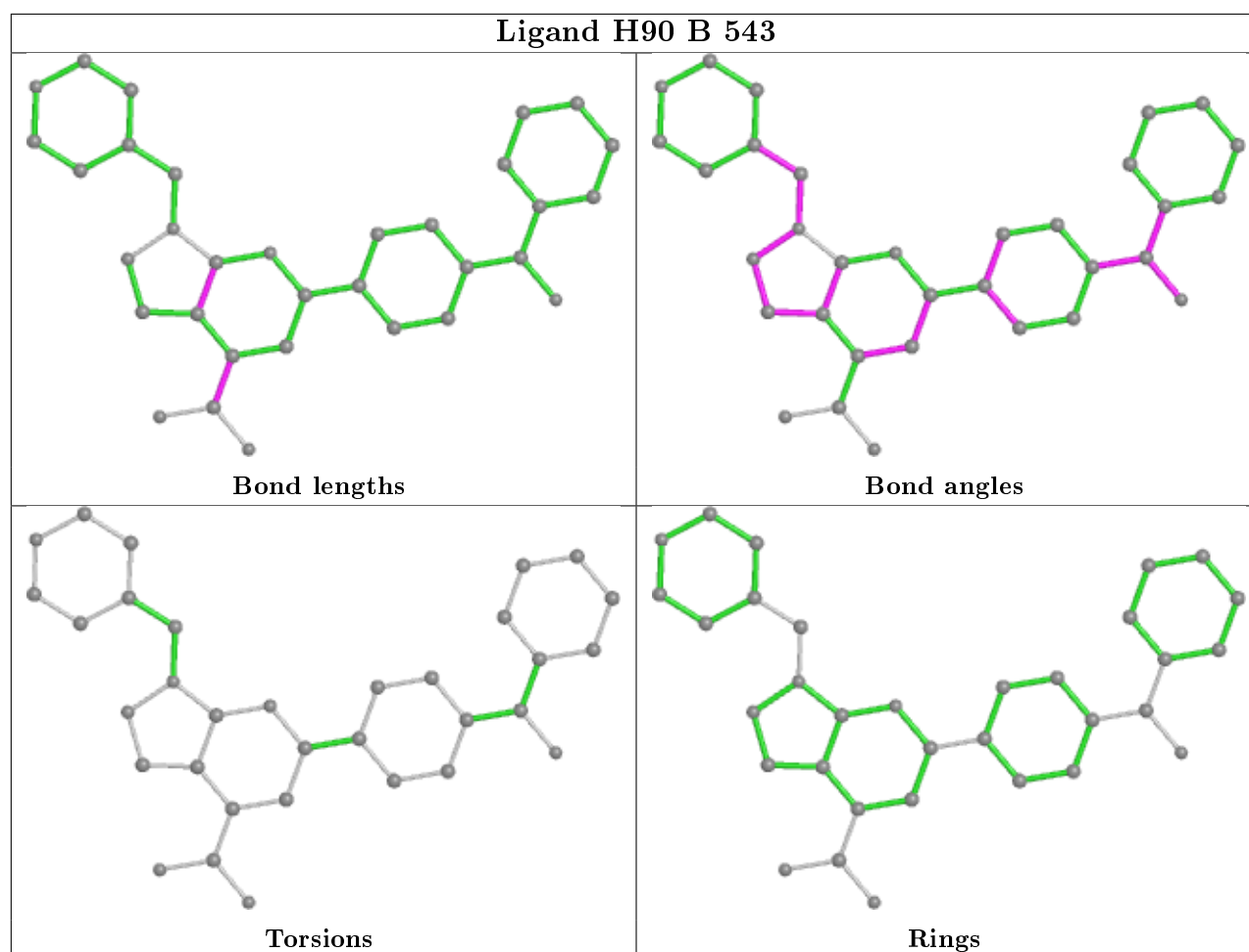
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	548	MPD	1	0
2	A	543	H90	3	0
2	B	543	H90	2	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.

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	433/544 (79%)	-0.03	16 (3%) 41 48	27, 37, 67, 84	0
1	B	436/544 (80%)	-0.16	10 (2%) 60 65	27, 39, 59, 76	0
All	All	869/1088 (79%)	-0.09	26 (2%) 50 56	27, 38, 64, 84	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	3.6
1	A	143	PHE	3.5
1	A	150	VAL	3.4
1	B	180	PHE	3.2
1	A	164	ALA	3.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

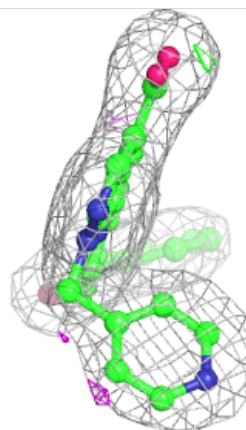
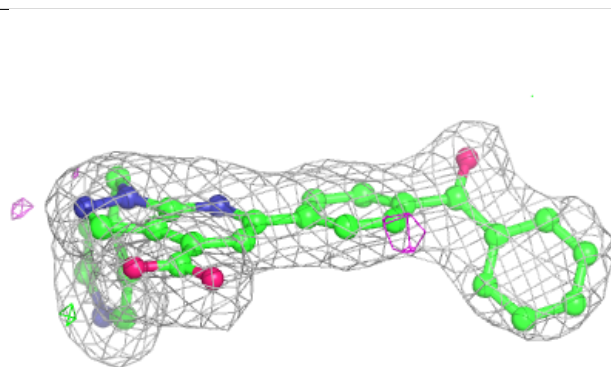
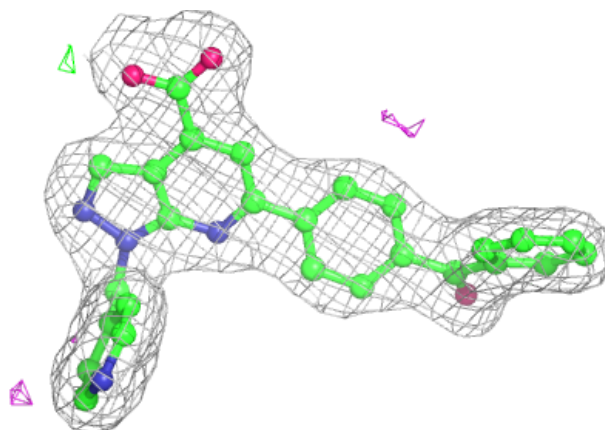
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	546	1/1	0.86	0.06	69,69,69,69	0
3	CA	A	547	1/1	0.88	0.16	73,73,73,73	0
3	CA	B	545	1/1	0.88	0.07	77,77,77,77	0
5	MRD	B	547	8/8	0.94	0.16	43,48,57,60	0
4	MPD	A	548	8/8	0.94	0.18	33,45,50,54	0
2	H90	A	543	33/33	0.96	0.14	22,33,46,48	0
3	CA	A	544	1/1	0.96	0.10	42,42,42,42	0
3	CA	B	544	1/1	0.97	0.10	48,48,48,48	0
2	H90	B	543	33/33	0.97	0.12	25,32,41,46	0
3	CA	A	546	1/1	0.98	0.10	35,35,35,35	0
3	CA	A	545	1/1	0.99	0.08	40,40,40,40	0

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.

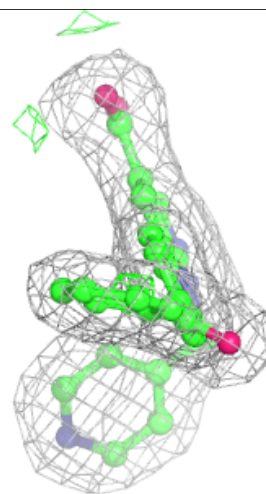
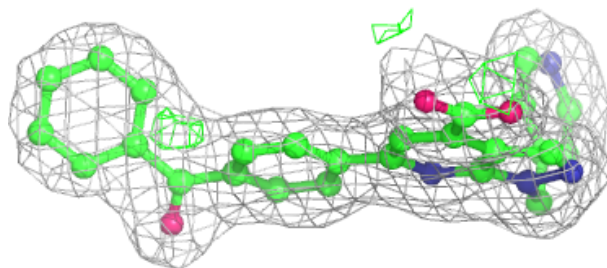
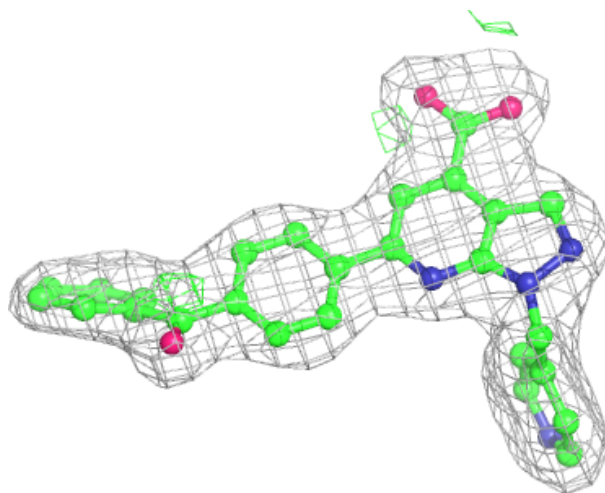
Electron density around H90 A 543:

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 H90 B 543:

$2mF_o-DF_c$ (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.