



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 PM UTC

PDB ID : 3U17 / pdb_00003u17
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 Full wwPDB X-ray Structure 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/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

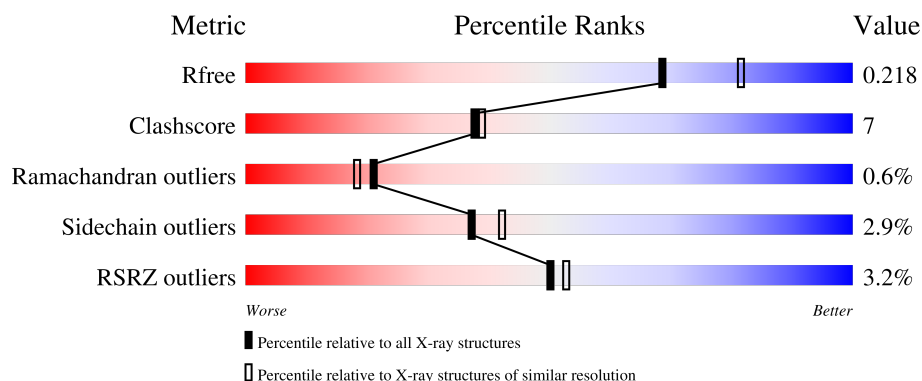
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	544	
1	B	544	

2 Entry composition

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.

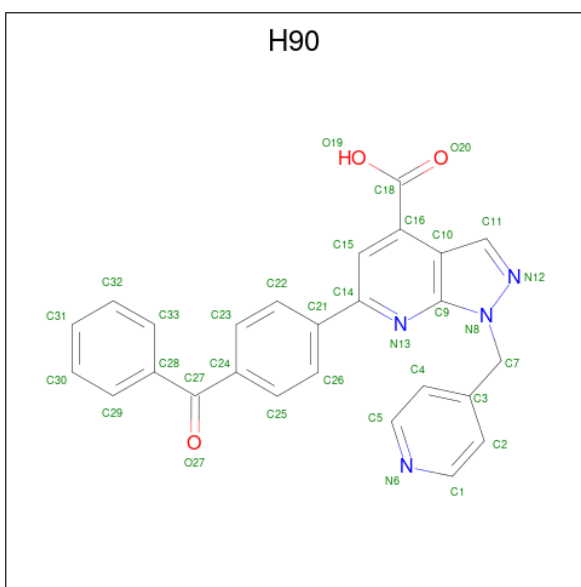
- Molecule 1 is a protein called Peptide arylation enzyme.

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: 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 (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



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

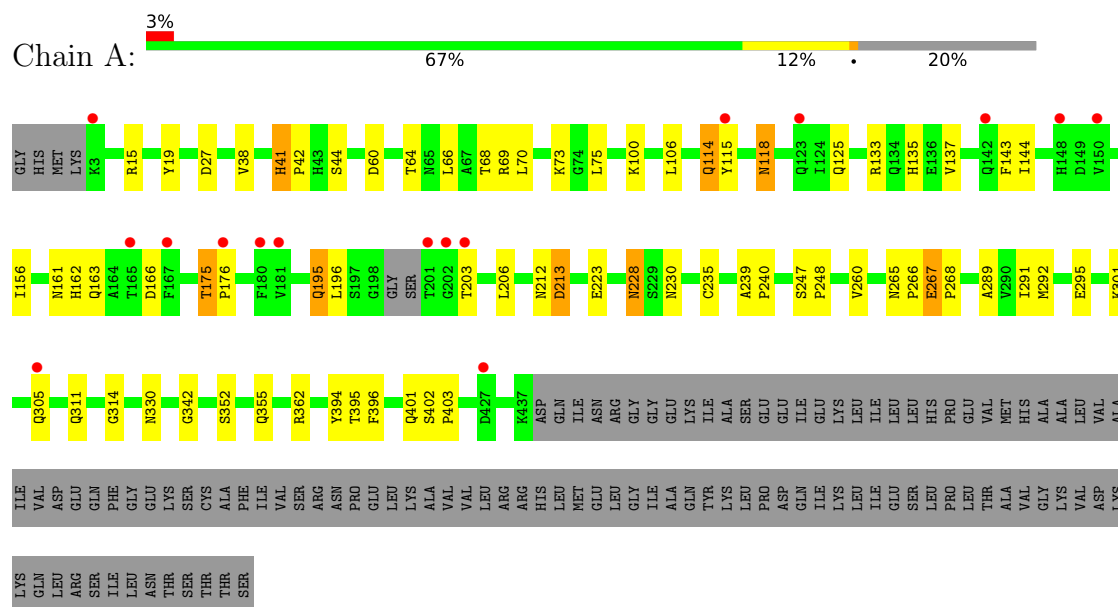
- Molecule 6 is water.

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

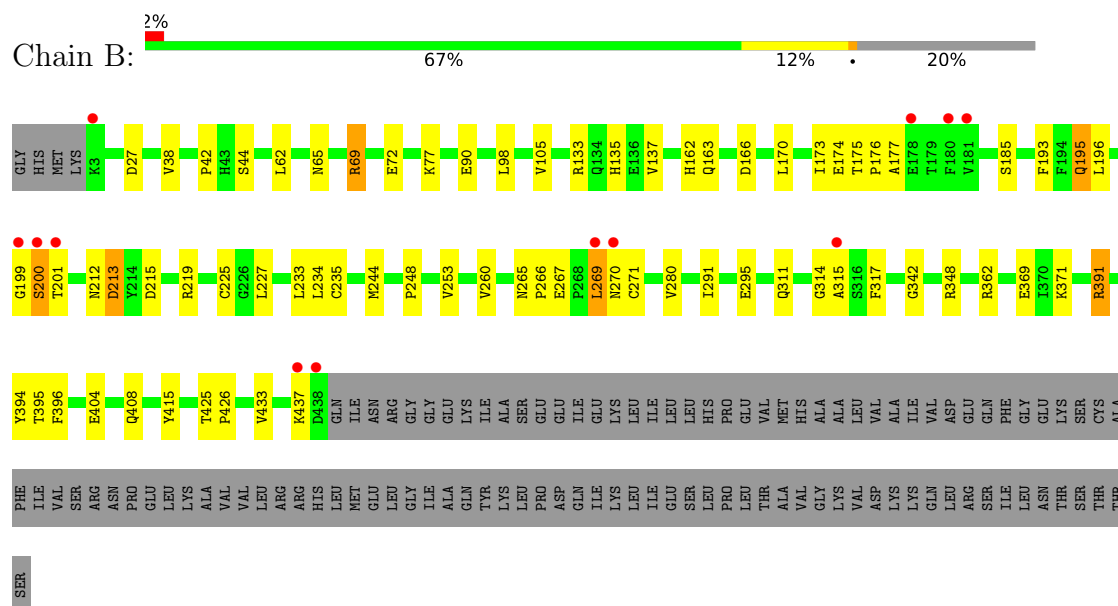
3 Residue-property plots [i](#)

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: Peptide arylation enzyme



• Molecule 1: Peptide arylation enzyme



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 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.1 (40.00-2.10) 90.1 (40.00-2.10)	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 , 0.218	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 , 38.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/3461	0.78	5/4711 (0.1%)
1	B	0.45	0/3471	0.75	2/4728 (0.0%)
All	All	0.44	0/6932	0.76	7/9439 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLU	CA-C-N	5.48	124.67	118.97
1	A	267	GLU	C-N-CA	5.48	124.67	118.97
1	A	247	SER	N-CA-C	5.28	118.24	109.79
1	B	317	PHE	CA-C-N	5.25	125.17	119.76
1	B	317	PHE	C-N-CA	5.25	125.17	119.76
1	A	41	HIS	CA-C-N	5.01	125.03	119.32
1	A	41	HIS	C-N-CA	5.01	125.03	119.32

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	3382	0	3302	48	0
1	B	3389	0	3292	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	95	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.

All (95) 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
1:A:352:SER:H	1:A:355:GLN:HE21	1.31	0.78
1:B:248:PRO:HD3	1:B:311:GLN:HE22	1.50	0.77
1:B:248:PRO:HD3	1:B:311:GLN:NE2	2.04	0.72
1:B:213:ASP:HB2	1:B:394:TYR:HA	1.72	0.71
1:A:228:ASN:ND2	1:A:230:ASN:H	1.90	0.68
1:A:235[B]:CYS:SG	1:A:260:VAL:HG13	2.33	0.67
1:A:195:GLN:HE21	1:A:196:LEU:H	1.44	0.66
1:B:235[B]:CYS:SG	1:B:260:VAL:HG13	2.38	0.62
1:A:213:ASP:HB2	1:A:394:TYR:HA	1.82	0.61
1:B:90:GLU:OE2	1:B:170:LEU:HD21	2.00	0.61
1:B:269:LEU:H	1:B:269:LEU:CD1	2.14	0.61
1:B:133:ARG:HG3	1:B:163:GLN:HG2	1.84	0.60
1:B:200:SER:HB3	6:B:584:HOH:O	1.99	0.60
1:A:228:ASN:HD22	1:A:228:ASN:C	2.10	0.60
1:B:225:CYS:SG	1:B:248:PRO:HG3	2.45	0.57
1:B:174:GLU:HG2	1:B:175:THR:HG23	1.87	0.56
1:A:15:ARG:HD2	1:A:19:TYR:OH	2.06	0.55
1:B:269:LEU:HD12	1:B:269:LEU:N	2.20	0.55
1:A:64:THR:O	1:A:68:THR:HG23	2.07	0.53
1:B:38:VAL:O	1:B:42:PRO:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:543:H90:H2	2:A:543:H90:C9	2.37	0.53
1:B:72:GLU:OE1	1:B:177:ALA:HB1	2.08	0.53
1:B:265:ASN:HB2	1:B:266:PRO:CD	2.38	0.52
1:A:352:SER:H	1:A:355:GLN:NE2	2.04	0.52
1:B:348:ARG:HG2	1:B:362:ARG:NH2	2.26	0.51
1:B:314:GLY:HA2	2:B:543:H90:C10	2.40	0.51
1:B:437:LYS:N	1:B:437:LYS:HD3	2.26	0.51
1:A:60:ASP:OD2	1:A:100:LYS:NZ	2.44	0.51
1:B:65:ASN:O	1:B:69:ARG:HG2	2.11	0.50
2:B:543:H90:H2	2:B:543:H90:C9	2.41	0.50
1:A:115:TYR:OH	1:B:291:ILE:HG22	2.12	0.50
1:B:135:HIS:CE1	1:B:137:VAL:HG23	2.47	0.50
1:B:267:GLU:HB3	1:B:269:LEU:HD13	1.94	0.49
1:A:163:GLN:O	1:A:166:ASP:HB2	2.12	0.49
1:A:144:ILE:HG12	6:A:715:HOH:O	2.12	0.49
1:A:291:ILE:O	1:A:295:GLU:HG2	2.13	0.49
1:B:235[B]:CYS:SG	1:B:260:VAL:CG1	3.01	0.49
1:B:266:PRO:HA	1:B:271:CYS:SG	2.53	0.48
1:A:228:ASN:HD22	1:A:230:ASN:N	2.05	0.48
1:A:305[A]:GLN:NE2	1:A:330:ASN:HD22	1.94	0.47
1:A:248:PRO:HD3	1:A:311:GLN:NE2	2.30	0.47
1:A:118:ASN:ND2	1:A:143:PHE:HE1	2.13	0.47
1:B:233:LEU:HB3	1:B:253:VAL:HG21	1.96	0.47
1:A:289:ALA:HA	1:A:292:MET:HE2	1.96	0.47
1:B:135:HIS:HE1	1:B:137:VAL:HG23	1.80	0.47
1:B:234:LEU:HB2	1:B:280:VAL:HG11	1.97	0.47
1:A:235[B]:CYS:SG	1:A:260:VAL:CG1	3.04	0.46
1:A:38:VAL:O	1:A:42:PRO:HG3	2.16	0.45
1:B:369:GLU:OE1	1:B:391:ARG:HD2	2.16	0.45
1:B:199:GLY:O	1:B:200:SER:O	2.35	0.45
1:A:175:THR:HA	1:A:176:PRO:HD3	1.81	0.45
4:A:548:MPD:HM2	4:A:548:MPD:H4	1.74	0.44
1:B:62:LEU:HD22	1:B:173:ILE:HG22	1.98	0.44
1:B:215:ASP:O	1:B:219:ARG:HG3	2.17	0.44
1:A:66:LEU:O	1:A:70:LEU:HG	2.18	0.44
1:B:65:ASN:OD1	1:B:176:PRO:HG3	2.18	0.44
1:A:133:ARG:HB2	1:A:161:ASN:O	2.18	0.44
1:B:105:VAL:O	1:B:193:PHE:HB2	2.18	0.43
1:A:228:ASN:ND2	1:A:228:ASN:C	2.76	0.43
1:A:195:GLN:NE2	1:A:196:LEU:H	2.15	0.43
1:A:314:GLY:HA2	2:A:543:H90:C10	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLY:HA3	1:A:395:THR:HA	1.99	0.43
1:B:195:GLN:HE21	1:B:196:LEU:H	1.66	0.43
1:B:342:GLY:HA3	1:B:395:THR:HA	2.01	0.43
1:A:265:ASN:HB2	1:A:266:PRO:CD	2.49	0.43
1:B:371:LYS:HE2	1:B:415:TYR:CG	2.54	0.43
1:A:73:LYS:HG2	1:A:156:ILE:HD11	2.01	0.43
1:B:162:HIS:HB2	1:B:166:ASP:HB2	2.01	0.43
1:B:404:GLU:O	1:B:408:GLN:HG2	2.19	0.43
1:A:75:LEU:HD11	1:A:156:ILE:HD12	2.01	0.42
1:A:248:PRO:HD3	1:A:311:GLN:HE22	1.83	0.42
1:B:227:LEU:HD11	1:B:248:PRO:HB2	2.01	0.42
1:A:314:GLY:HA2	2:A:543:H90:C16	2.50	0.42
1:B:425:THR:HB	1:B:426:PRO:HD2	2.01	0.42
1:B:244:MET:HE3	1:B:244:MET:HA	2.02	0.42
1:A:135:HIS:HE1	1:A:137:VAL:HG23	1.86	0.41
1:A:362:ARG:NE	6:A:578:HOH:O	2.27	0.41
1:B:77:LYS:HE3	1:B:185:SER:O	2.20	0.41
1:A:27:ASP:HA	1:A:212:ASN:OD1	2.21	0.41
1:A:239:ALA:N	1:A:240:PRO:CD	2.83	0.41
1:A:41:HIS:HB2	1:A:44:SER:OG	2.21	0.41
1:A:267:GLU:HA	1:A:268:PRO:HD3	1.89	0.41
1:A:162:HIS:HB2	1:A:166:ASP:HB2	2.02	0.41
1:A:114:GLN:O	1:A:118:ASN:HB2	2.21	0.41
1:B:69:ARG:HG2	1:B:69:ARG:H	1.56	0.41
1:B:98:LEU:HD13	1:B:105:VAL:HB	2.02	0.41
1:B:27:ASP:HA	1:B:212:ASN:OD1	2.21	0.40
1:A:402:SER:N	1:A:403:PRO:HD3	2.36	0.40
1:A:118:ASN:HD22	1:A:143:PHE:HE1	1.67	0.40
1:A:305[A]:GLN:HE22	1:A:330:ASN:ND2	1.95	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 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%)	43	44
1	B	420/544 (77%)	407 (97%)	9 (2%)	4 (1%)	12	9
All	All	851/1088 (78%)	827 (97%)	19 (2%)	5 (1%)	21	18

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%)	354 (97%)	12 (3%)	33	37
1	B	366/472 (78%)	357 (98%)	9 (2%)	42	48
All	All	732/944 (78%)	711 (97%)	21 (3%)	37	42

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	114	GLN
1	A	118	ASN
1	A	125	GLN
1	A	175	THR
1	A	195	GLN
1	A	206	LEU
1	A	213	ASP
1	A	223	GLU
1	A	228	ASN
1	A	301	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	396	PHE
1	B	44	SER
1	B	69	ARG
1	B	195	GLN
1	B	201	THR
1	B	213	ASP
1	B	295	GLU
1	B	391	ARG
1	B	396	PHE
1	B	433	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	21	ASN
1	A	118	ASN
1	A	195	GLN
1	A	228	ASN
1	A	230	ASN
1	A	270	ASN
1	A	303	GLN
1	A	355	GLN
1	B	17	GLN
1	B	18	HIS
1	B	21	ASN
1	B	41	HIS
1	B	53	GLN
1	B	142	GLN
1	B	195	GLN
1	B	230	ASN
1	B	276	GLN
1	B	405	HIS
1	B	408	GLN

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](#)

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	$\# Z > 2$
5	MRD	B	547	-	7,7,7	0.37	0	9,10,10	0.54	0
4	MPD	A	548	-	7,7,7	0.38	0	9,10,10	0.57	0
2	H90	B	543	-	37,37,37	1.39	3 (8%)	50,52,52	2.70	14 (28%)
2	H90	A	543	-	37,37,37	1.41	4 (10%)	50,52,52	2.87	10 (20%)

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
5	MRD	B	547	-	-	3/5/5/5	-
4	MPD	A	548	-	-	1/5/5/5	-
2	H90	B	543	-	-	0/20/20/20	0/5/5/5
2	H90	A	543	-	-	0/20/20/20	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	543	H90	N8-N12	5.14	1.41	1.37
2	B	543	H90	N8-N12	4.87	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	543	H90	C11-N12	3.88	1.36	1.32
2	A	543	H90	C9-N8	-3.65	1.32	1.35
2	A	543	H90	C11-N12	3.08	1.35	1.32
2	B	543	H90	C9-N8	-2.81	1.33	1.35
2	A	543	H90	C7-C3	2.17	1.55	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	543	H90	N13-C9-N8	9.59	132.42	126.31
2	A	543	H90	C10-C11-N12	-8.99	104.55	111.38
2	B	543	H90	N13-C9-N8	8.81	131.92	126.31
2	B	543	H90	C10-C11-N12	-8.53	104.90	111.38
2	A	543	H90	C9-C10-C11	7.63	110.88	104.42
2	B	543	H90	C9-C10-C11	7.27	110.57	104.42
2	A	543	H90	C3-C7-N8	-5.94	103.98	112.51
2	B	543	H90	C10-C9-N13	-5.52	123.05	126.56
2	A	543	H90	C10-C9-N13	-5.32	123.18	126.56
2	A	543	H90	C10-C9-N8	-4.82	104.40	107.26
2	B	543	H90	C3-C7-N8	-4.76	105.67	112.51
2	A	543	H90	C7-N8-C9	4.57	130.71	127.81
2	B	543	H90	C10-C9-N8	-3.83	104.99	107.26
2	B	543	H90	C7-N8-C9	3.51	130.04	127.81
2	A	543	H90	C7-N8-N12	-3.30	116.61	120.80
2	A	543	H90	C9-N8-N12	3.25	112.58	110.98
2	A	543	H90	C11-N12-N8	3.06	107.58	106.06
2	B	543	H90	C9-N8-N12	2.72	112.32	110.98
2	B	543	H90	O27-C27-C24	-2.70	115.83	120.15
2	B	543	H90	C7-N8-N12	-2.50	117.63	120.80
2	B	543	H90	C26-C21-C22	2.41	121.99	117.68
2	B	543	H90	C11-N12-N8	2.30	107.20	106.06
2	B	543	H90	C25-C24-C23	2.20	121.37	118.57
2	B	543	H90	C23-C22-C21	-2.12	118.40	121.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

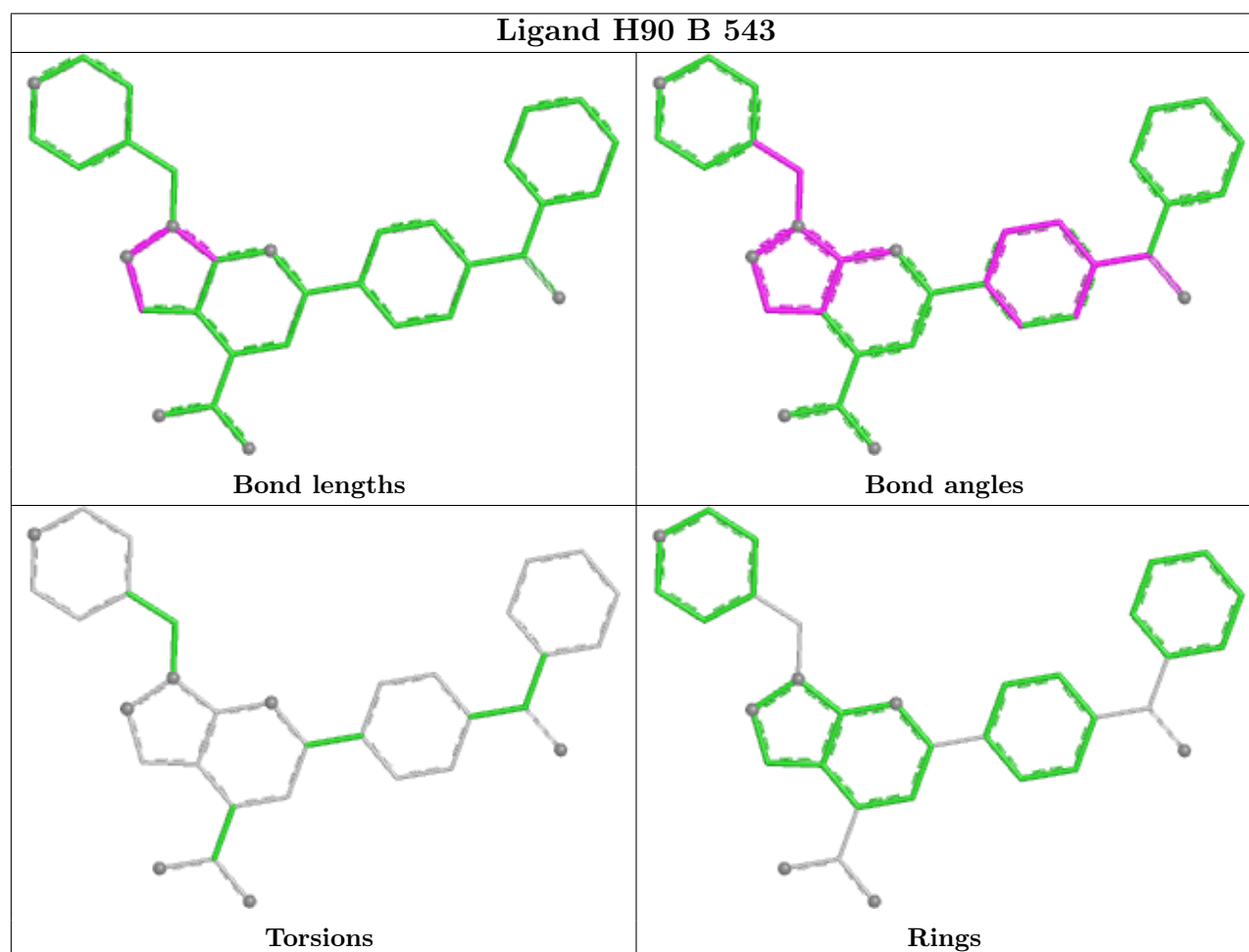
Mol	Chain	Res	Type	Atoms
5	B	547	MRD	O2-C2-C3-C4
5	B	547	MRD	C2-C3-C4-C5
4	A	548	MPD	O2-C2-C3-C4
5	B	547	MRD	C2-C3-C4-O4

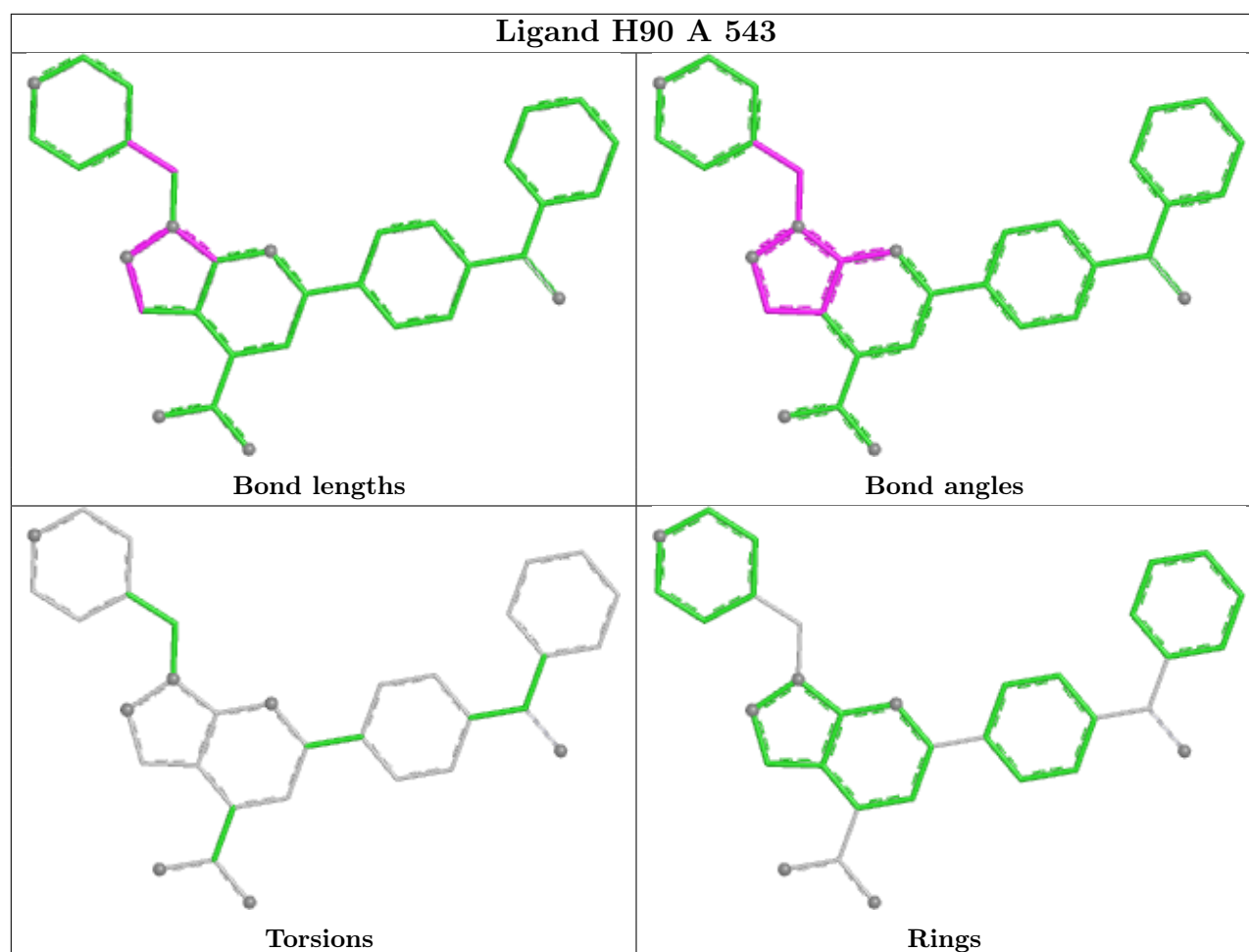
There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

6.1 Protein, DNA and RNA chains

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%)	0.01	16 (3%)	45	47	19, 37, 67, 84	2 (0%)
1	B	436/544 (80%)	0.01	12 (2%)	55	57	23, 39, 59, 76	1 (0%)
All	All	869/1088 (79%)	0.01	28 (3%)	50	53	19, 38, 64, 84	3 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	5.5
1	A	201	THR	5.5
1	A	202	GLY	5.0
1	B	270	ASN	4.1
1	A	305[A]	GLN	3.8
1	B	315	ALA	3.6
1	A	115	TYR	3.3
1	A	148	HIS	3.1
1	A	142	GLN	2.9
1	B	201	THR	2.8
1	B	180	PHE	2.7
1	A	3	LYS	2.7
1	A	167	PHE	2.7
1	B	437	LYS	2.7
1	B	438	ASP	2.6
1	A	180	PHE	2.5
1	A	150	VAL	2.5
1	A	181	VAL	2.4
1	A	176	PRO	2.3
1	A	203	THR	2.3
1	A	427	ASP	2.2
1	B	3	LYS	2.2
1	A	165	THR	2.2
1	A	123	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	SER	2.1
1	B	181	VAL	2.1
1	B	178	GLU	2.0
1	B	199	GLY	2.0

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](#)

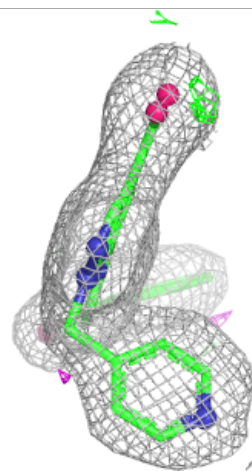
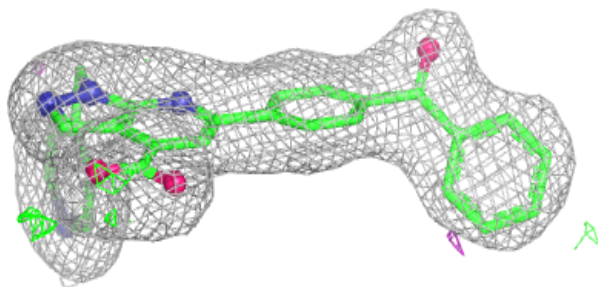
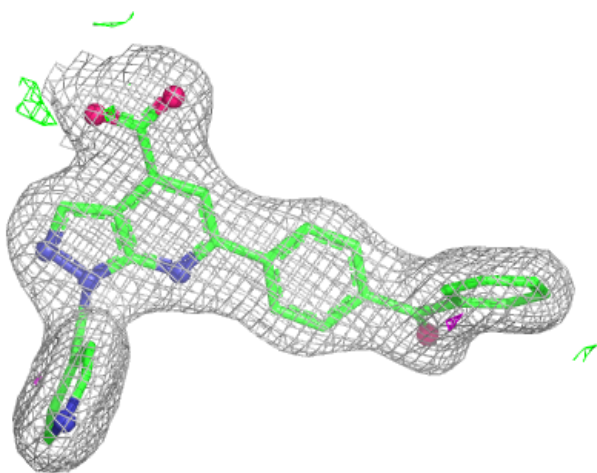
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	547	1/1	0.78	0.13	73,73,73,73	0
3	CA	B	545	1/1	0.87	0.10	77,77,77,77	0
5	MRD	B	547	8/8	0.89	0.16	43,48,57,60	0
4	MPD	A	548	8/8	0.90	0.13	33,45,50,54	0
3	CA	B	546	1/1	0.92	0.07	69,69,69,69	0
3	CA	A	544	1/1	0.96	0.06	42,42,42,42	0
2	H90	A	543	33/33	0.96	0.07	22,33,46,48	0
2	H90	B	543	33/33	0.97	0.06	25,32,41,46	0
3	CA	B	544	1/1	0.97	0.05	48,48,48,48	0
3	CA	A	546	1/1	0.98	0.04	35,35,35,35	0
3	CA	A	545	1/1	0.99	0.03	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.

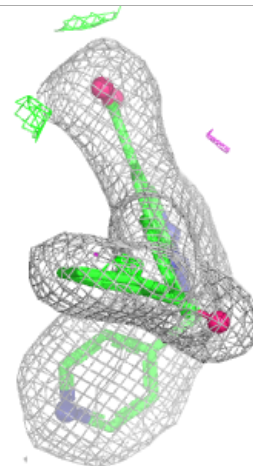
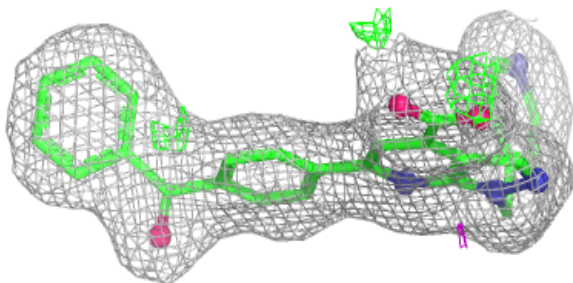
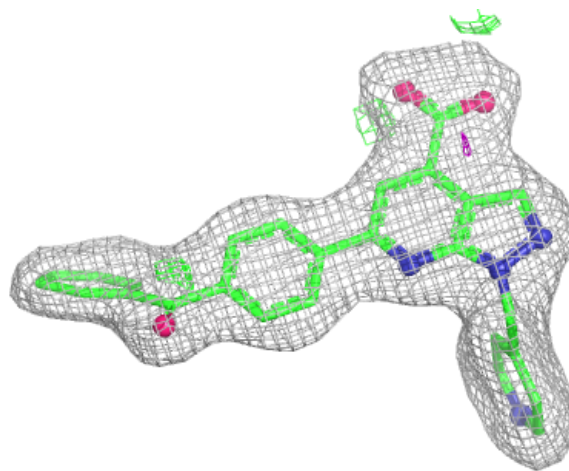
Electron density around H90 A 543:

$2mF_o-DF_c$ (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.