



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:20 PM UTC

PDB ID : 6KHE / pdb_00006khe
Title : Crystal structure of CLK2 in complex with CX-4945
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Deposited on : 2019-07-15
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

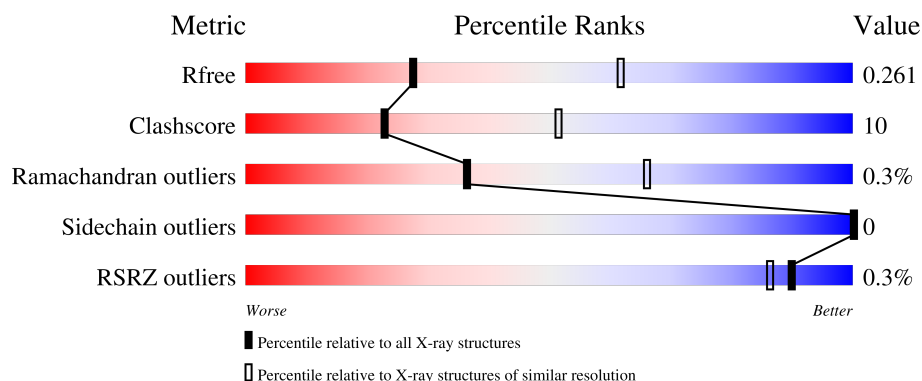
1 Overall quality at a glance

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	499	51% 17% 31%

2 Entry composition [i](#)

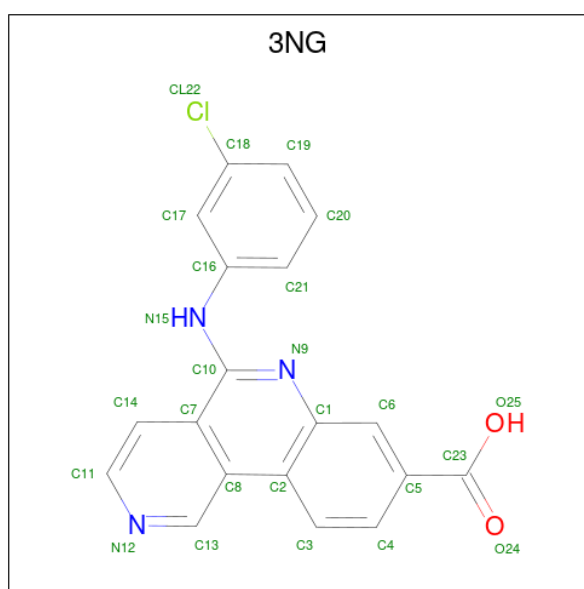
There are 3 unique types of molecules in this entry. The entry contains 2907 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dual specificity protein kinase CLK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2848	1811	505	518	14			

- Molecule 2 is 5-[(3-chlorophenyl)amino]benzo[c][2,6]naphthyridine-8-carboxylic acid (CCD ID: 3NG) (formula: C₁₉H₁₂ClN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total	O	0
			34	34	

- Molecule 1: Dual specificity protein kinase CLK2

ARG	V364	D219	ARG	ASP	MET
ASP			ARG	ARG	PRO
ILE	I371	V227	ARG	ARG	HIS
SER	F372	Q228	ARG	SER	PRO
ARG	E373		SER	ASP	ARG
		Y235	ARG	ARG	ARG
	V376		THR	ARG	TYR
	G377	M239	PHE	VAL	HIS
	F378		SER	TYR	ARG
		E244	ARG	ASP	SER
	T383		SER	ARG	GLU
		T250	SER	ARG	ARG
	R387	F251	SER	TYR	GLY
		D252	GLN	CYS	GLY
	N392	F253	HIS	GLY	ARG
		L254	SER	SER	GLY
	F414	K255	SER	TYR	SER
	Y415	D256	ARG	ARG	TYR
	R416		ARG	ARG	ARG
		Y259	ALA	ASN	GLU
	L419		LYS	ASP	GLU
	D420	Y262	VAL	TYR	HIS
	W421			TYR	ARG
	D422	M270	E144	SER	ARG
	E423			SER	SER
		Q273	H150	ASP	ARG
			L151	ARG	ARG
	G428	H288	L152	GLY	LYS
	R429	T289	Y153	ASP	HIS
		D290		ALA	LYS
	R432			ALA	ARG
			L159	TYR	ARG
	R439	P293	Q190	TYR	ARG
				ASP	ARG
	I456	I296	E164	THR	SER
	E457		I165	TYR	ARG
	S458	L305		ARG	TRP
	W459		T168	SER	SER
	E461	N308	L169	SER	SER
			G170	TYR	SER
		E315	E171	GLU	ASP
	P464	R316		TYR	ARG
		S317	F174	GLN	THR
	R467	V318	G175	ARG	ARG
	L468		R176	GLU	ARG
	T469	T321	V177	ASN	ARG
			V178	SER	ARG
	E472	R324	Q179	SER	ARG
		V325		TYR	GLU
		V326	H183	ARG	ASP
	R483			SER	ASP
	A484	G329	K193	GLN	TYR
	E485	S330	I194	ARG	HIS
PRO			I195	SER	VAL
ASN		F333	V198	SER	ARG
LYS		D334		ARG	ARG
LEU		H335	E203	LYS	ARG
TRP		E336		HIS	SER
ASP			E208	ARG	SER
SER		E351		ARG	TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 75.63Å 161.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.46 – 2.80 40.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.46-2.80) 99.6 (40.46-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998: ???	Depositor
R, R_{free}	0.196 , 0.261 0.196 , 0.261	Depositor DCC
R_{free} test set	1218 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2907	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: 3NG

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	0.39	0/2920	0.60	0/3944

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	2848	0	2767	59	1
2	A	25	0	11	1	0
3	A	34	0	0	4	0
All	All	2907	0	2778	59	1

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 10.

The worst 5 of 59 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:351:GLU:HG2	1:A:464:PRO:HG3	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:HB	1:A:392:MET:CE	1.98	0.94
1:A:383:THR:HB	1:A:392:MET:HE1	1.58	0.84
1:A:289:THR:HG22	1:A:330:SER:HB2	1.63	0.79
1:A:171:GLU:OE2	1:A:176:ARG:NH1	2.17	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:O	1:A:483:ARG:NH1[6_555]	1.88	0.32

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	340/499 (68%)	318 (94%)	21 (6%)	1 (0%)	36 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	VAL

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 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	308/459 (67%)	308 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	224	ASN
1	A	295	ASN
1	A	308	ASN

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](#)

1 ligand is 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$
2	3NG	A	1000	-	28,28,28	2.00	6 (21%)	39,40,40	4.55	12 (30%)

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
2	3NG	A	1000	-	-	2/8/8/8	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	3NG	C10-N15	4.99	1.43	1.36
2	A	1000	3NG	C7-C8	-4.61	1.34	1.42
2	A	1000	3NG	C10-C7	-4.04	1.39	1.44
2	A	1000	3NG	C10-N9	3.77	1.38	1.32
2	A	1000	3NG	C13-N12	2.34	1.36	1.32

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	3NG	C7-C10-N15	18.85	138.85	119.77
2	A	1000	3NG	N15-C10-N9	-17.99	102.57	118.55
2	A	1000	3NG	C14-C7-C10	-5.05	116.89	124.16
2	A	1000	3NG	C4-C5-C23	-3.34	113.77	120.37
2	A	1000	3NG	C10-C7-C8	3.24	121.41	117.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	3NG	C7-C10-N15-C16
2	A	1000	3NG	N9-C10-N15-C16

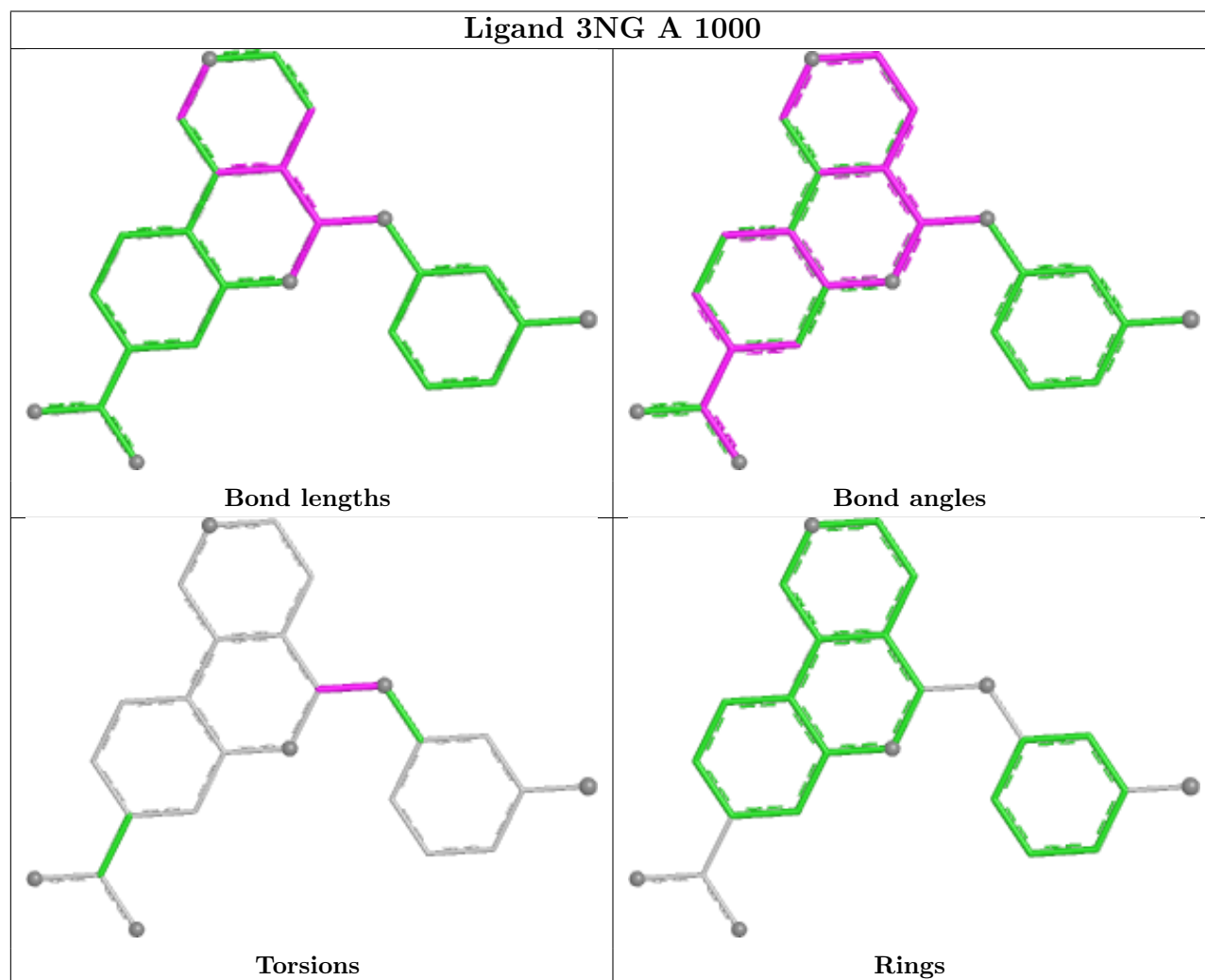
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	3NG	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.

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	342/499 (68%)	-0.15	1 (0%) 90 86	36, 50, 76, 103	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	TRP	2.3

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](#)

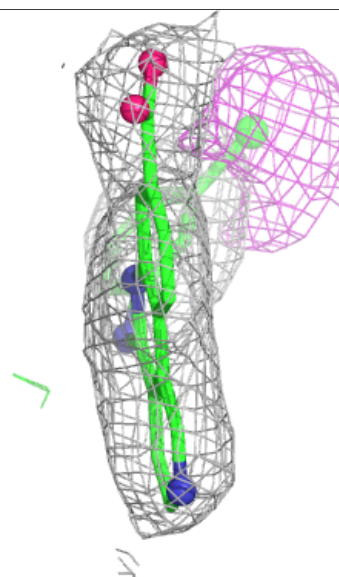
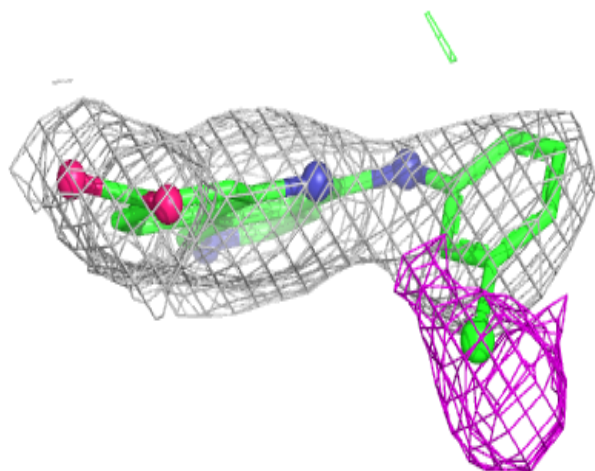
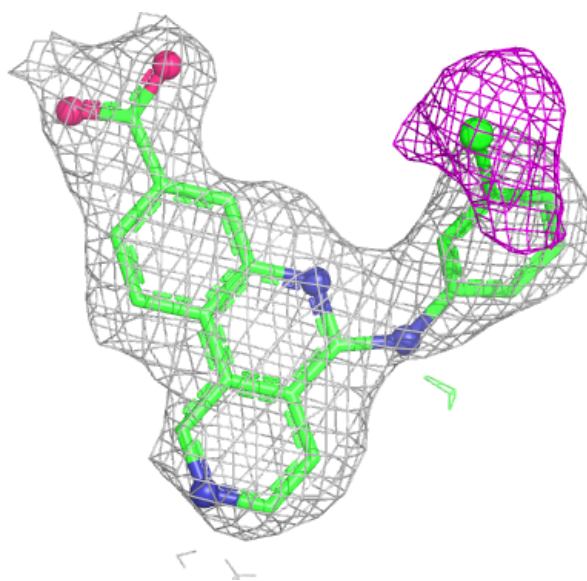
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	3NG	A	1000	25/25	0.87	0.13	44,53,63,88	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 3NG A 1000:

$2mF_o-DF_c$ (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.