



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:28 pm BST

PDB ID : 3NDM  
Title : Crystal structure of Rho-Associated Protein Kinase (ROCK1) with a potent isoquinolone derivative  
Authors : Li, X.  
Deposited on : 2010-06-07  
Resolution : 3.30 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](mailto: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.

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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	:	2.11
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)	:	2.11

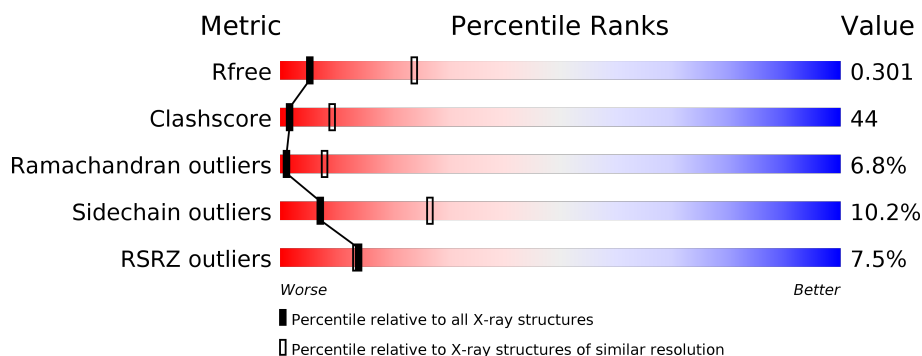
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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	415	
1	B	415	
1	C	415	
1	D	415	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12746 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.

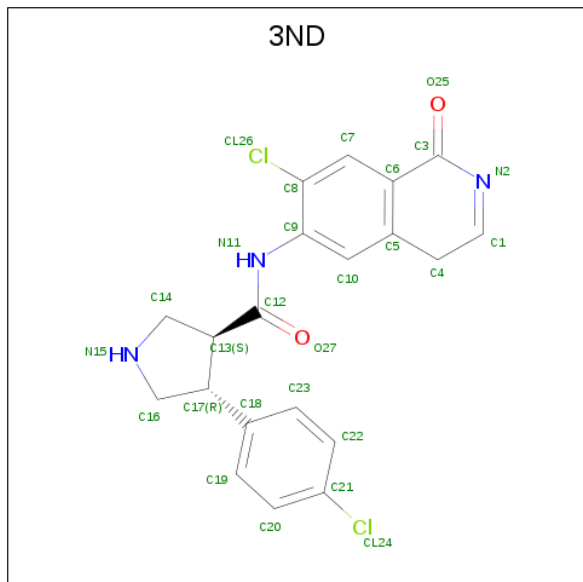
- Molecule 1 is a protein called Rho-Associated Protein Kinase (ROCK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3128	2005	517	584	22			
1	B	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			
1	C	371	Total	C	N	O	S	0	0	0
			3028	1944	493	569	22			
1	D	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q13464
A	2	SER	-	EXPRESSION TAG	UNP Q13464
A	3	LEU	-	EXPRESSION TAG	UNP Q13464
A	4	HIS	-	EXPRESSION TAG	UNP Q13464
A	5	MET	-	EXPRESSION TAG	UNP Q13464
B	1	GLY	-	EXPRESSION TAG	UNP Q13464
B	2	SER	-	EXPRESSION TAG	UNP Q13464
B	3	LEU	-	EXPRESSION TAG	UNP Q13464
B	4	HIS	-	EXPRESSION TAG	UNP Q13464
B	5	MET	-	EXPRESSION TAG	UNP Q13464
C	1	GLY	-	EXPRESSION TAG	UNP Q13464
C	2	SER	-	EXPRESSION TAG	UNP Q13464
C	3	LEU	-	EXPRESSION TAG	UNP Q13464
C	4	HIS	-	EXPRESSION TAG	UNP Q13464
C	5	MET	-	EXPRESSION TAG	UNP Q13464
D	1	GLY	-	EXPRESSION TAG	UNP Q13464
D	2	SER	-	EXPRESSION TAG	UNP Q13464
D	3	LEU	-	EXPRESSION TAG	UNP Q13464
D	4	HIS	-	EXPRESSION TAG	UNP Q13464
D	5	MET	-	EXPRESSION TAG	UNP Q13464

- Molecule 2 is (3S,4R)-N-(7-chloro-1-oxo-1,4-dihydroisoquinolin-6-yl)-4-(4-chlorophenyl)pyrrolidine-3-carboxamide (three-letter code: 3ND) (formula: C<sub>20</sub>H<sub>17</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		

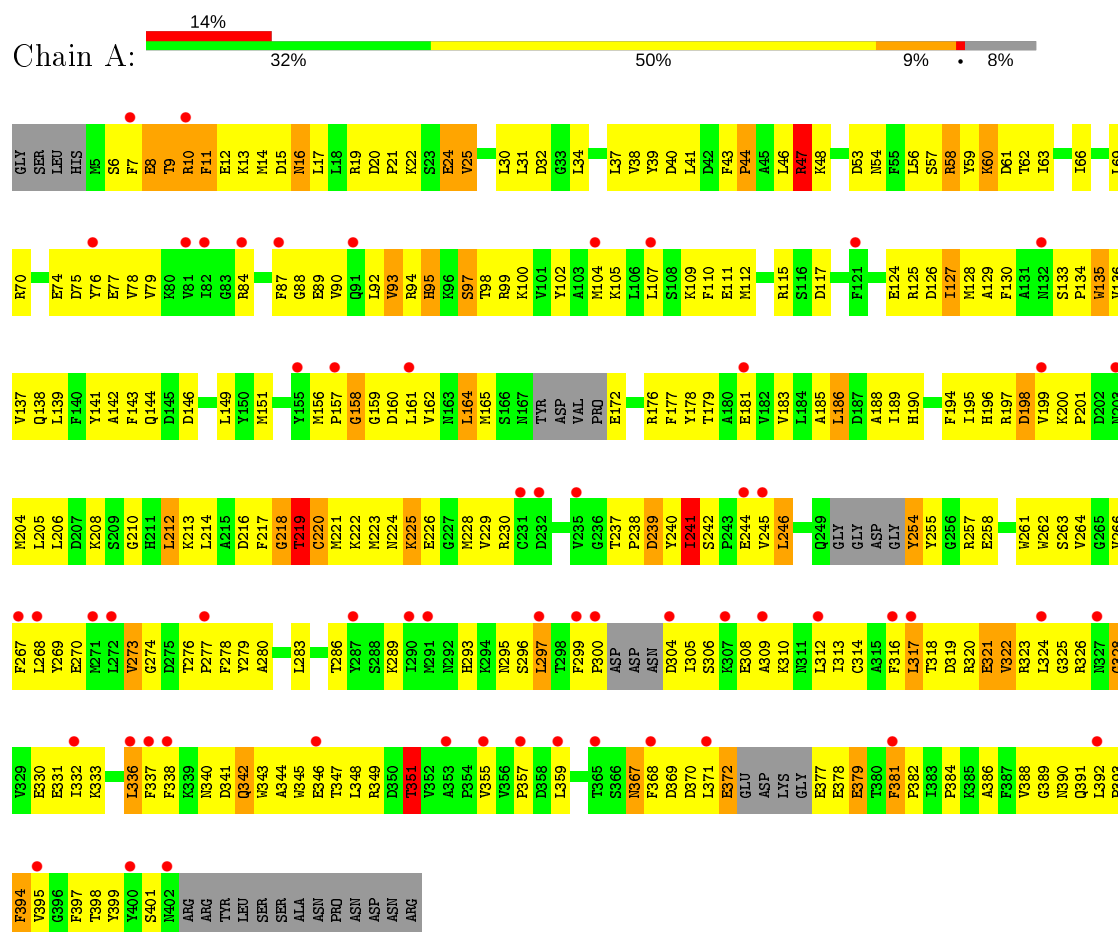
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		
3	C	15	Total	O	0	0
			15	15		
3	D	14	Total	O	0	0
			14	14		

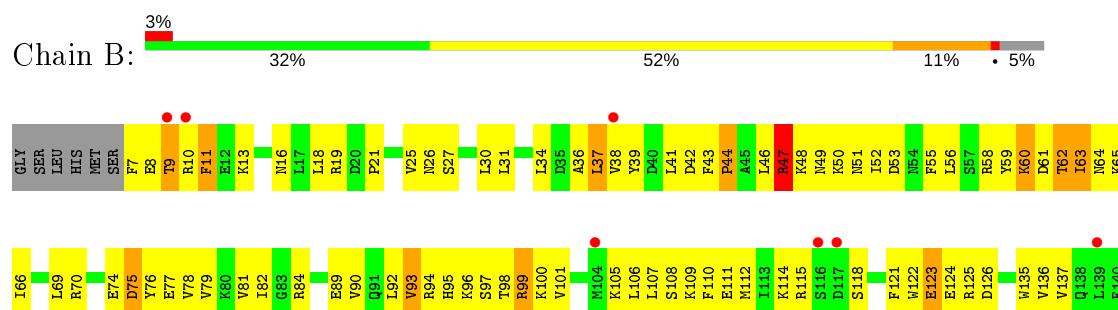
### 3 Residue-property plots [i](#)

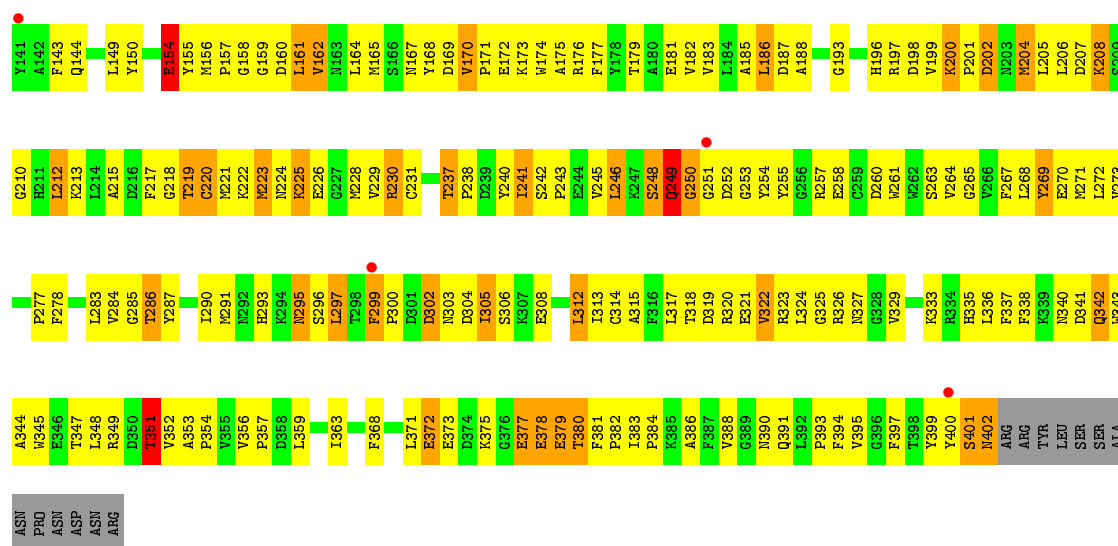
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Rho-Associated Protein Kinase (ROCK1)

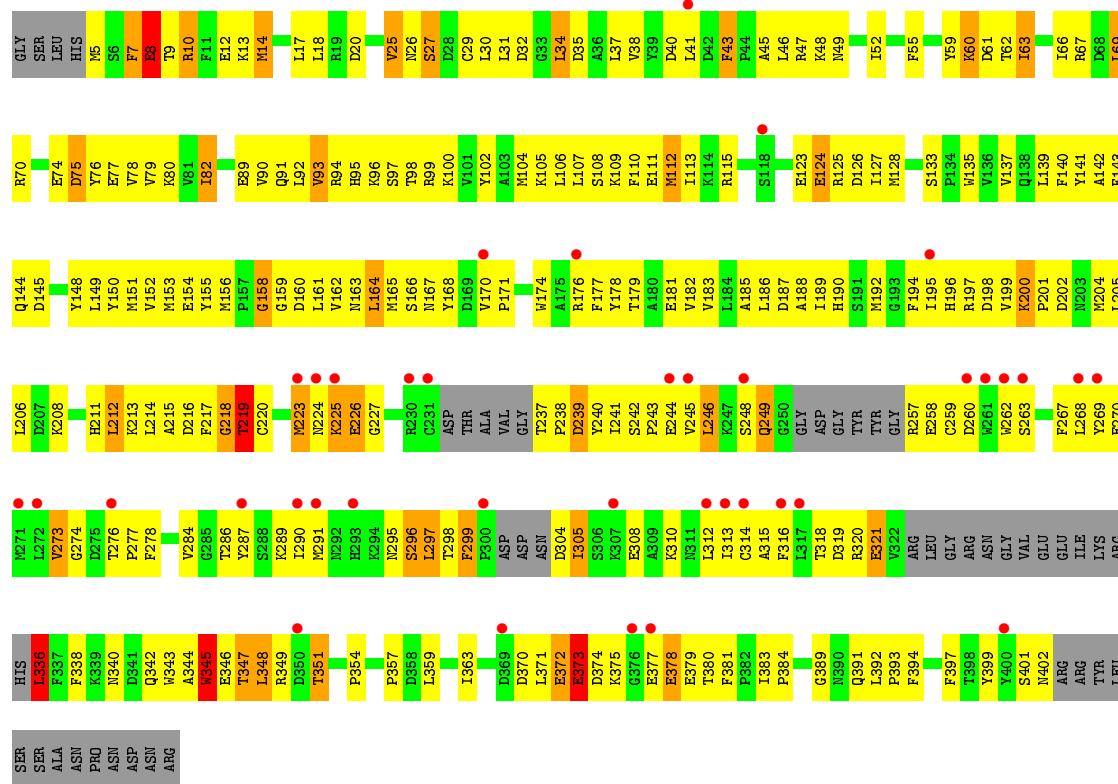


#### • Molecule 1: Rho-Associated Protein Kinase (ROCK1)

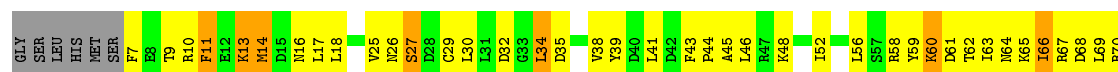




### • Molecule 1: Rho-Associated Protein Kinase (ROCK1)



### • Molecule 1: Rho-Associated Protein Kinase (ROCK1)



ASN	D341	L268	P201	Q138	W71
PRO	Q342	Y269	D202	L139	K72
ASN	W343	E270	N203	F140	
ASP	A344	M271	N204		D75
ASN	W345	L272	L205	F143	Y76
ASN	E346	V273	L206	G144	
ARG	T347		D207	D145	
	L348	P277	K208	D146	V79
	R349	F278	S209	R147	K80
	D350		G210	Y148	V81
	T351	D281	H211		I82
		L212		V152	G83
	P354	S282		M153	R84
	V355	L283	D216	E154	
	V356	V284	F217	Y155	E89
	P357	T286	G218	M156	V90
		Y287	T219	P157	Q91
	D362	S288	C220	G158	L92
	I363	K289	N221	G159	V93
	D364	I290	K222	D160	R94
	T365		M223	L161	H95
		K294	N224	V162	A96
	F368	N295	K225	N163	S97
	D369	S296	E226	L164	T98
	D370	L297	G227	M165	R99
	L371	T298	V229	S166	K100
	E372	F299	R230	M167	V101
	E373	P300	C231	Y168	
	D374			D169	M104
		N303	V235	V170	K105
	E377	D304		P171	L106
	E378	I305	G236	L107	L107
	E379	S306	T237	S108	S108
	T380	K307	P238	A109	A109
	F381		D239	W174	F110
		L312	Y240	A175	E111
	I383	I313	I241	R176	M112
	P384	G314	S242	F177	I113
	K385	A315	F243	Y178	K114
	A386	F316	E244	T179	K115
	F387	L317	V245	A180	S116
	V388	T318	V245	E181	D117
	G389	K247	L246	V182	S118
	N390	V222	K247	V183	A119
	Q391	K323	S248	L184	F120
	L392	L324	Q249	A185	F121
	P393	G325	G250	L186	F122
		R326	G251	D187	W123
		N327	D252	A188	E124
	F397	G328	G253	I189	R125
		V329		H190	D126
	Y400	E330	R257	S191	I127
	N402	E331		M192	M128
	ARG	I332	D260	G193	A129
	ARG	K333	W261	F194	F130
	TYR		W262	I195	
	LEU	F337	S263	H196	S133
	SER	F338	V264	R197	F134
	SER	K339	G265	D198	W135
	ALA	N340	V266	V199	V136
			F267	K200	V137

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.78 Å   83.55 Å   177.96 Å 90.00°   119.95°   90.00°	Depositor
Resolution (Å)	42.53 – 3.30 44.72 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.53-3.30) 99.6 (44.72-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.32 Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, $R_{free}$	0.241 , 0.310 0.232 , 0.301	Depositor DCC
$R_{free}$ test set	1402 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 160.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3ND

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	0/3199	0.57	0/4314
1	B	0.55	0/3299	0.67	0/4457
1	C	0.49	0/3098	0.62	1/4180 (0.0%)
1	D	0.56	0/3299	0.67	0/4457
All	All	0.50	0/12895	0.63	1/17408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	LEU	CA-CB-CG	-5.52	102.60	115.30

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	3128	0	3048	269	0
1	B	3222	0	3120	282	0
1	C	3028	0	2943	304	0
1	D	3222	0	3120	292	0
2	B	27	0	17	7	0
2	C	27	0	17	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	17	5	0
3	A	20	0	0	5	0
3	B	16	0	0	3	0
3	C	15	0	0	5	0
3	D	14	0	0	1	0
All	All	12746	0	12282	1105	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 44.

The worst 5 of 1105 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:66:ILE:HD11	1:B:25:VAL:HG21	1.35	1.08
1:A:399:TYR:CE2	1:A:401:SER:HB2	1.91	1.04
1:A:230:ARG:HH21	1:A:254:TYR:HB2	1.23	1.02
1:C:78:VAL:HA	1:C:93:VAL:HG12	1.42	1.00
1:B:38:VAL:HG21	1:B:63:ILE:HG13	1.41	0.99

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	373/415 (90%)	282 (76%)	65 (17%)	26 (7%)	1	7
1	B	394/415 (95%)	294 (75%)	70 (18%)	30 (8%)	1	6
1	C	361/415 (87%)	268 (74%)	67 (19%)	26 (7%)	1	7
1	D	394/415 (95%)	286 (73%)	86 (22%)	22 (6%)	2	11
All	All	1522/1660 (92%)	1130 (74%)	288 (19%)	104 (7%)	1	8

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	99	ARG
1	A	273	VAL
1	A	351	THR
1	B	60	LYS

### 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	343/369 (93%)	307 (90%)	36 (10%)	7	25
1	B	352/369 (95%)	312 (89%)	40 (11%)	5	22
1	C	334/369 (90%)	302 (90%)	32 (10%)	8	29
1	D	352/369 (95%)	319 (91%)	33 (9%)	8	30
All	All	1381/1476 (94%)	1240 (90%)	141 (10%)	7	27

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	ILE
1	C	14	MET
1	D	288	SER
1	B	319	ASP
1	B	372	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	ASN
1	C	211	HIS
1	D	327	ASN
1	C	190	HIS
1	C	292	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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
2	3ND	C	900	-	28,30,30	1.10	2 (7%)	38,43,43	1.88	8 (21%)
2	3ND	D	900	-	28,30,30	1.09	2 (7%)	38,43,43	1.92	8 (21%)
2	3ND	B	900	-	28,30,30	1.16	3 (10%)	38,43,43	1.95	8 (21%)

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	3ND	C	900	-	-	3/12/32/32	0/3/4/4
2	3ND	D	900	-	-	2/12/32/32	0/3/4/4
2	3ND	B	900	-	-	2/12/32/32	0/3/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	3ND	C1-N2	3.36	1.36	1.28
2	B	900	3ND	C1-N2	3.36	1.36	1.28
2	C	900	3ND	C1-N2	3.02	1.35	1.28
2	C	900	3ND	C3-N2	-2.65	1.33	1.38
2	B	900	3ND	C18-C17	-2.48	1.48	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	3ND	C18-C17-C13	-6.49	100.92	114.64
2	D	900	3ND	C18-C17-C13	-6.18	101.57	114.64
2	C	900	3ND	C18-C17-C13	-5.67	102.64	114.64
2	D	900	3ND	C13-C12-N11	5.43	121.18	114.50
2	C	900	3ND	C13-C12-N11	5.13	120.82	114.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	3ND	O27-C12-C13-C17
2	D	900	3ND	O27-C12-C13-C17
2	B	900	3ND	O27-C12-C13-C17
2	C	900	3ND	N11-C12-C13-C17
2	D	900	3ND	N11-C12-C13-C17

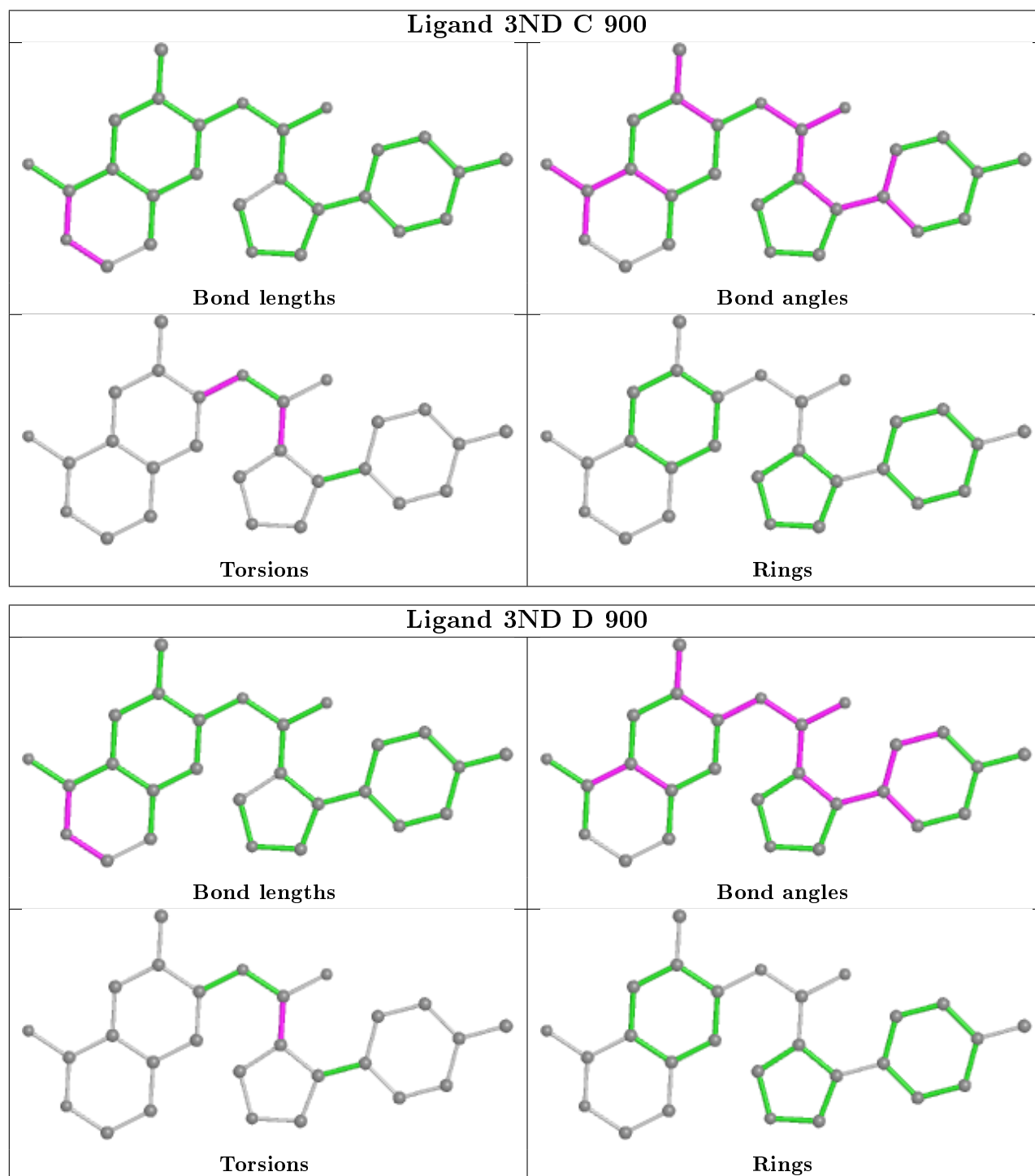
There are no ring outliers.

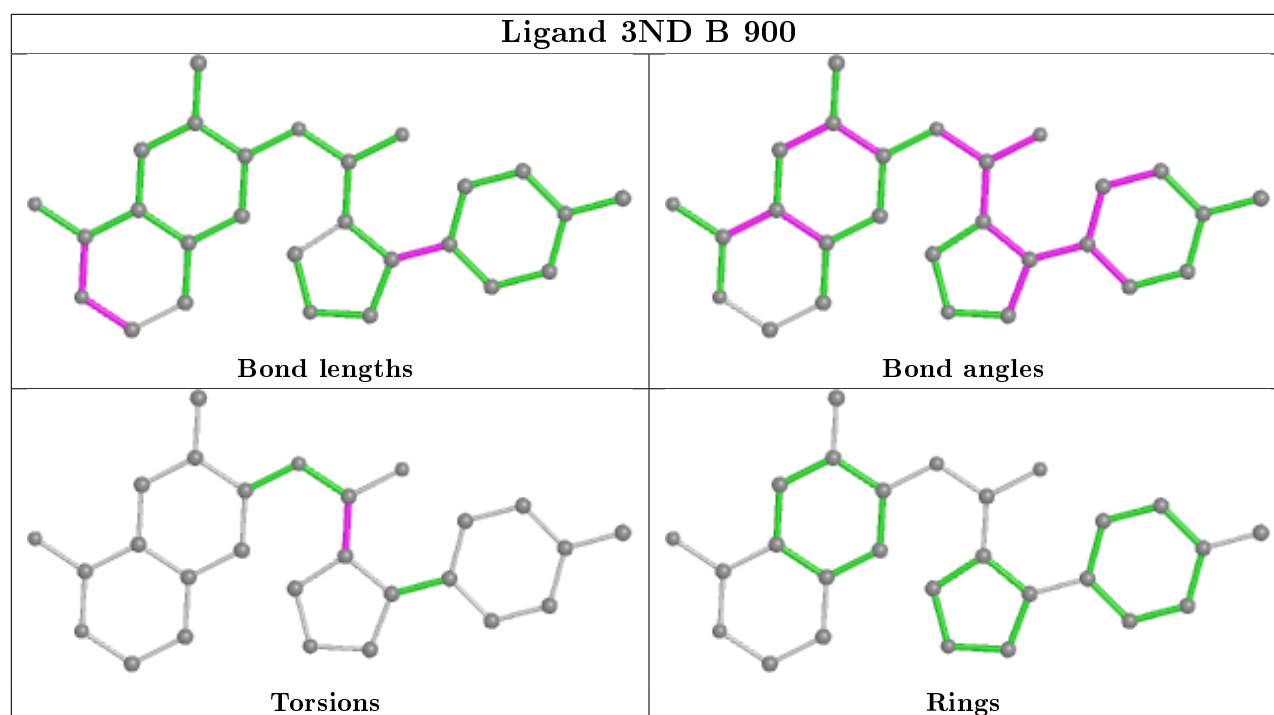
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	3ND	4	0
2	D	900	3ND	5	0
2	B	900	3ND	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	383/415 (92%)	0.74	59 (15%) <b>2</b> <b>2</b>	102, 200, 300, 366	0
1	B	396/415 (95%)	0.16	11 (2%) 53 51	83, 143, 237, 329	0
1	C	371/415 (89%)	0.44	38 (10%) <b>6</b> <b>6</b>	88, 168, 274, 403	0
1	D	396/415 (95%)	0.18	8 (2%) 65 64	82, 153, 232, 336	0
All	All	1546/1660 (93%)	0.38	116 (7%) <b>14</b> <b>13</b>	82, 164, 271, 403	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	TYR	6.8
1	A	245	VAL	5.0
1	C	260	ASP	4.9
1	A	336	LEU	4.7
1	A	353	ALA	4.7

### 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 carbohydrates 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, 95<sup>th</sup> 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.

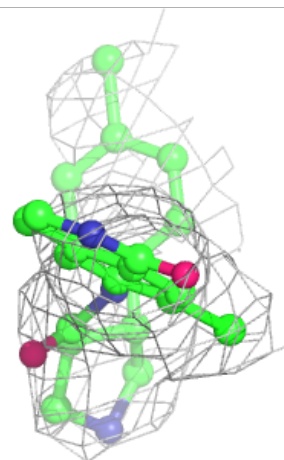
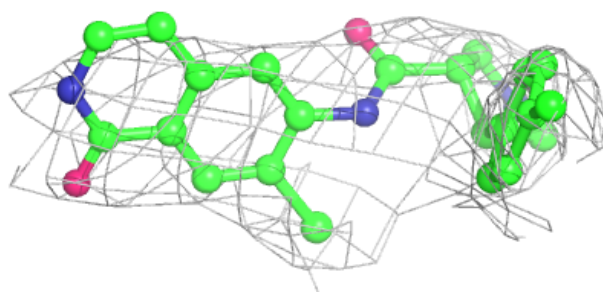
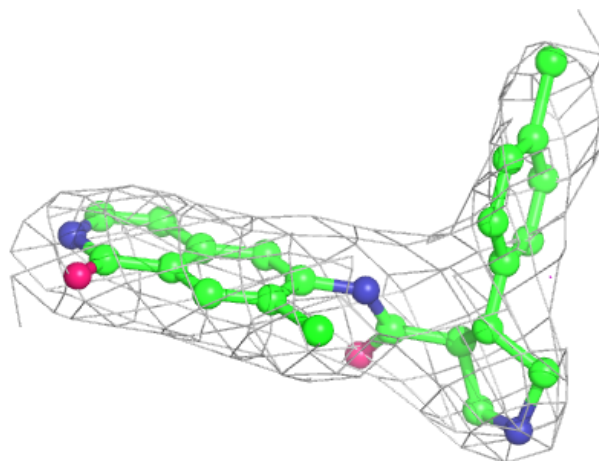


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3ND	D	900	27/27	0.88	0.33	150,150,150,150	0
2	3ND	B	900	27/27	0.90	0.28	142,142,142,142	0
2	3ND	C	900	27/27	0.92	0.25	138,138,138,138	0

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.

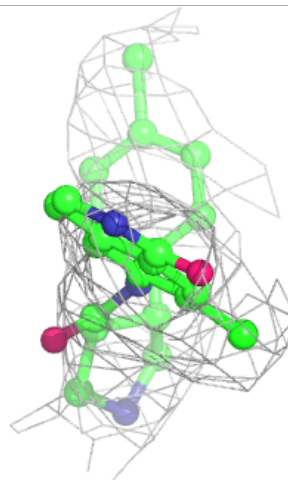
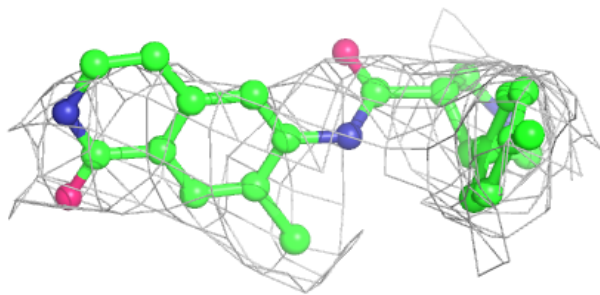
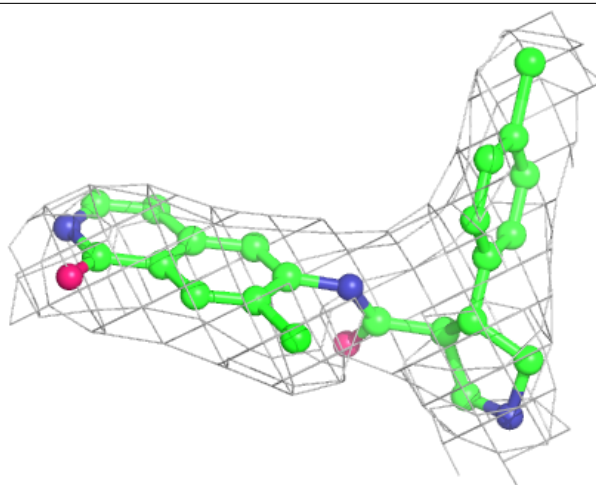
**Electron density around 3ND D 900:**

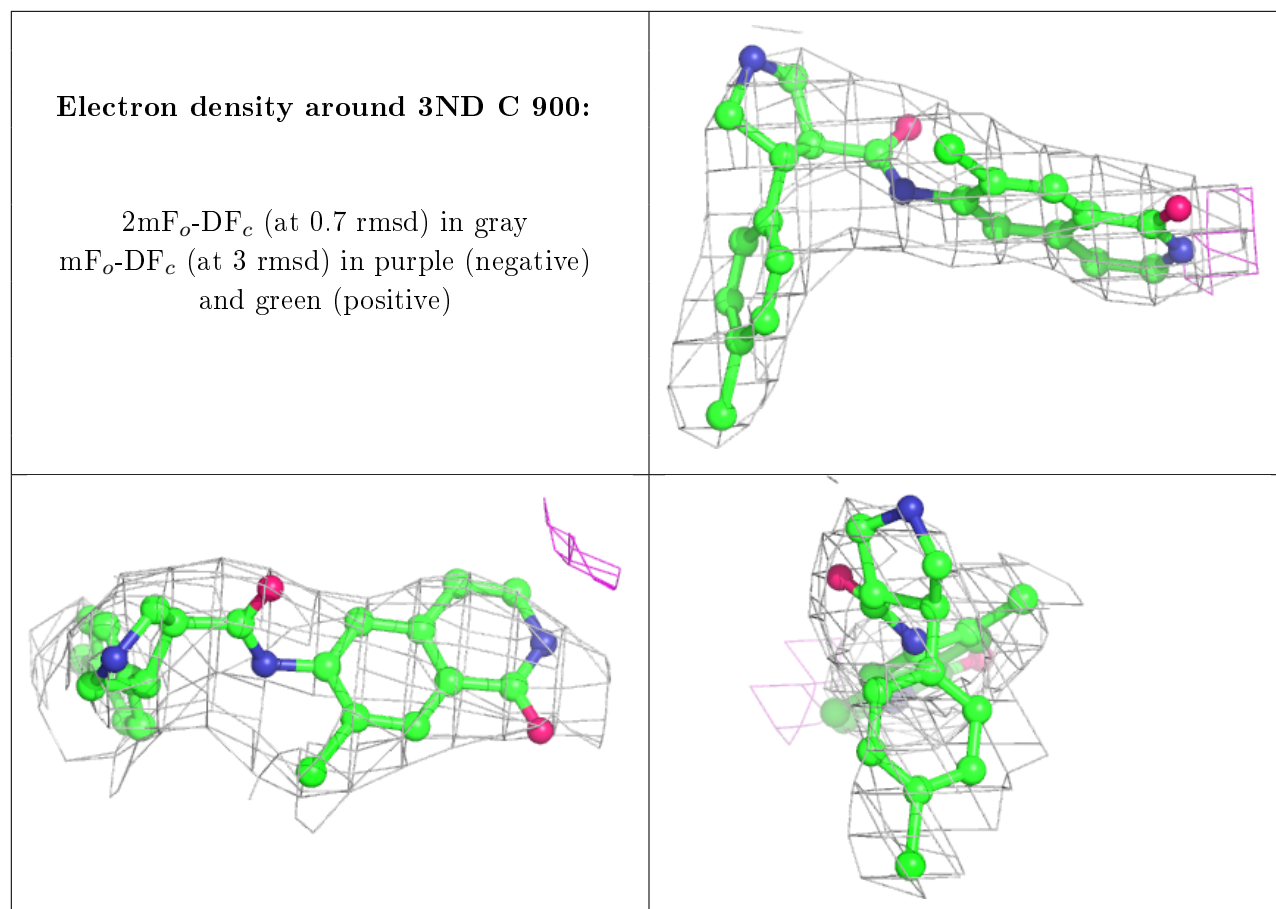
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 3ND B 900:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.