

# wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 07:13 PM JST

PDB ID : 7VP9

Title : Crystal structure of human ClpP in complex with ZG111

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Deposited on : 2021-10-15

Resolution : 2.55 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 (i) 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 (1)) 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 : 2.36

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)

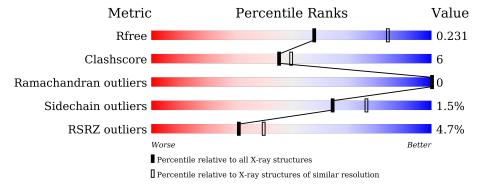
Validation Pipeline (wwPDB-VP) : 2.36

## 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 2.55 Å.

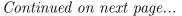
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
IVICUIC	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 <=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	221	69%	8% 23%					
1	В	221	5% 65%	12% 23%					
1	С	221	5% 62%	13% • 24%					
1	D	221	52%	24% • 23%					
1	Е	221	63%	13% • 23%					
1	F	221	60%	18% 23%					





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Mol	Chain	Length	Quality of chain					
1	G	221	66%	11% 23%				
1	Н	221	% <b>7</b> 6%	5% 19%				
1	I	221	71%	10% 19%				
1	J	221	71%	9% 19%				
1	K	221	71%	8% 20%				
1	L	221	74%	7% 19%				
1	M	221	7%	8% • 19%				
1	N	221	71%	10% 19%				



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19269 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.

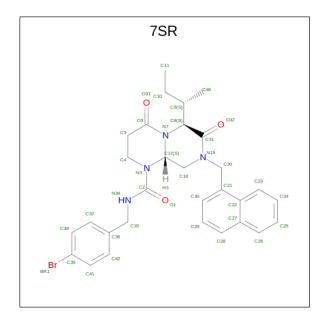
• Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	A	170	Total	С	N	О	S	0	0	0
1	11	170	1306	836	219	238	13	0	U	U
1	В	170	Total	$\mathbf{C}$	N	Ο	S	0	0	0
1	Б	110	1300	831	221	236	12	Ů,	0	U
1	С	168	Total	С	N	О	S	0	0	0
	C	100	1266	809	215	229	13	Ŭ	Ů,	Ů
1	D	170	Total	$\mathbf{C}$	N	Ο	S	0	0	0
	D	110	1288	821	220	235	12	0	0	U
1	E	171	Total	С	N	Ο	S	0	0	0
	L	111	1309	839	220	237	13	Ŭ	Ŭ	U
1	F	171	Total	С	N	Ο	S	0	0	0
1	1	111	1312	841	221	237	13		Ů,	
1	G	170	Total	С	N	Ο	S	0	0	0
1	G G	110	1314	843	219	239	13		ŭ	U
1	Н	180	Total	$\mathbf{C}$	N	O	S	0	0	0
1	11	100	1395	887	240	255	13		U	U
1	I	178	Total	С	N	O	S	0	0	0
1	1	170	1366	874	232	247	13		O	U
1	J	178	Total	$\mathbf{C}$	N	O	S	0	0	0
1	3	170	1360	870	227	250	13		0	U
1	K	176	Total	С	N	O	S	0	0	0
1	11	170	1334	857	225	239	13		U	U
1	L	179	Total	С	N	O	S	0	0	0
	ш	113	1385	882	237	254	12		U	U
1	M	179	Total	С	N	О	S	0	0	0
1	1V1	W   179	1358	866	230	249	13		U	U
1	N	170	Total	С	N	О	S	0	0	0
1	IN	179	1375	875	236	251	13	U	U	U

• Molecule 2 is (6S,9aS)-N-[(4-bromophenyl)methyl]-6-[(2S)-butan-2-yl]-8-(naphthalen-1-ylme thyl)-4,7-bis(oxidanylidene)-3,6,9,9a-tetrahydro-2H-pyrazino[1,2-a]pyrimidine-1-carboxa mide (three-letter code: 7SR) (formula: C<sub>30</sub>H<sub>33</sub>BrN<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by



depositor).



Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf
2	A	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	A	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	В	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	D	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	D	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	Е	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	G	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	Н	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	I	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	I	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	K	1	Total 38	Br 1	C 30	N 4	O 3	0	0
2	K	1	38	Br 1	C 30	N 4	O 3	0	0
2	L	1	Total 38	Br 1	C 30	N 4	O 3	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	N	1	Total	Br	С	N	О	0	0
	2   N	1	38	1	30	4	3	U	

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	Е	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	Н	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	В	3	Total O 3 3	0	0



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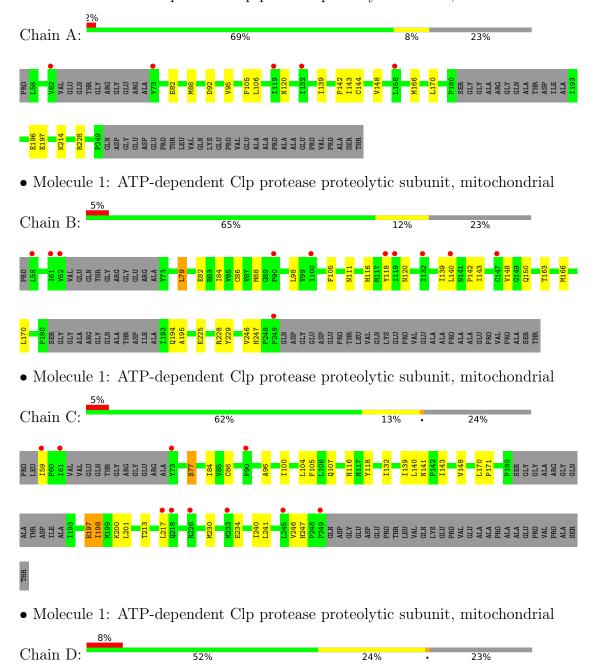
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	Н	7	Total O 7 7	0	0
4	I	13	Total O 13 13	0	0
4	J	10	Total O 10 10	0	0
4	K	4	Total O 4 4	0	0
4	L	2	Total O 2 2	0	0
4	M	3	Total O 3 3	0	0
4	N	3	Total O 3 3	0	0

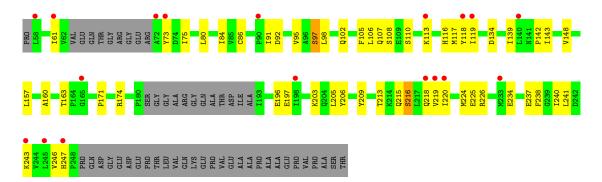


## 3 Residue-property plots (i)

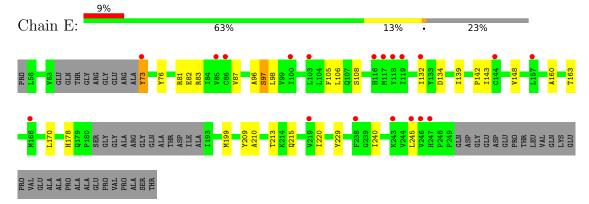
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-dependent Clp protease proteolytic subunit, mitochondrial

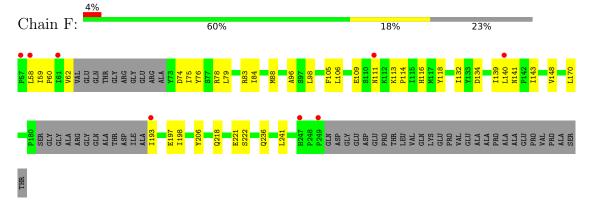




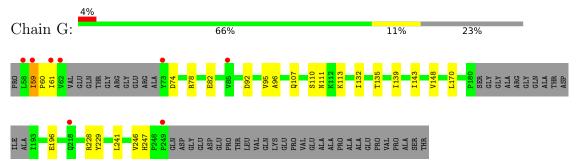
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

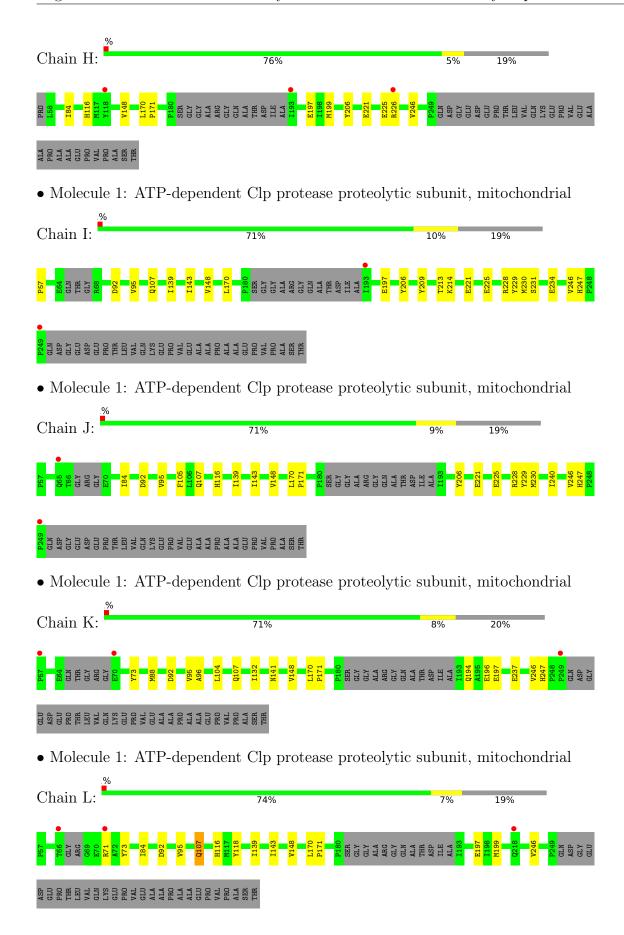


• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



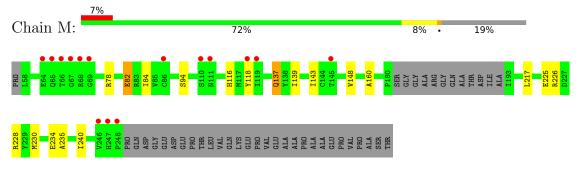
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



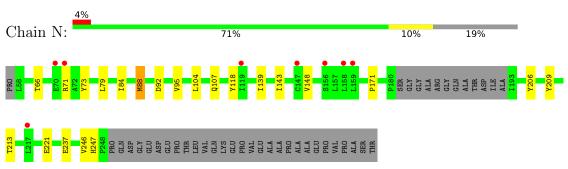




• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	103.81Å 97.41Å 146.69Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.63^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	28.84 - 2.55	Depositor
Resolution (A)	28.84 - 2.55	EDS
% Data completeness	95.2 (28.84-2.55)	Depositor
(in resolution range)	95.2 (28.84 - 2.55)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.85 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
Ρ. Р.	0.202 , $0.232$	Depositor
$R, R_{free}$	0.202 , $0.231$	DCC
$R_{free}$ test set	4637 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 50.9	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG, 7SR

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.34	0/1331	0.62	1/1805 (0.1%)	
1	В	0.38	0/1324	0.66	2/1795~(0.1%)	
1	С	0.48	0/1290	0.67	3/1749~(0.2%)	
1	D	0.44	0/1311	0.75	0/1779	
1	Е	0.43	0/1334	0.64	0/1810	
1	F	0.35	0/1337	0.59	1/1813 (0.1%)	
1	G	0.45	0/1339	0.56	0/1814	
1	Н	0.37	0/1421	0.54	0/1925	
1	I	0.39	0/1392	0.53	0/1886	
1	J	0.43	0/1386	0.56	0/1880	
1	K	0.47	0/1360	0.67	3/1846 (0.2%)	
1	L	0.46	0/1411	0.59	0/1911	
1	M	0.32	0/1383	0.60	1/1876 (0.1%)	
1	N	0.38	0/1400	0.59	0/1896	
All	All	0.41	0/19019	0.61	$11/25785 \ (0.0\%)$	

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	В	88	MET	CB-CA-C	-7.87	94.65	110.40
1	M	137	GLN	CA-CB-CG	7.28	129.41	113.40
1	K	88	MET	CA-CB-CG	7.25	125.62	113.30
1	A	214	LYS	CA-CB-CG	-6.15	99.87	113.40
1	В	88	MET	N-CA-CB	6.12	121.61	110.60

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	1306	0	1316	14	0
1	В	1300	0	1315	24	0
1	С	1266	0	1263	24	0
1	D	1288	0	1282	51	0
1	Ε	1309	0	1321	25	0
1	F	1312	0	1337	33	0
1	G	1314	0	1337	18	0
1	Н	1395	0	1416	8	0
1	I	1366	0	1386	15	0
1	J	1360	0	1360	12	0
1	K	1334	0	1339	9	0
1	L	1385	0	1402	9	0
1	M	1358	0	1358	15	0
1	N	1375	0	1390	17	0
2	A	76	0	0	4	0
2	В	38	0	0	1	0
2	D	76	0	0	8	0
2	Ε	38	0	0	1	0
2	G	38	0	0	1	0
2	Η	38	0	0	0	0
2	I	76	0	0	1	0
2	K	76	0	0	1	0
2	L	38	0	0	0	0
2	N	38	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Ε	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
4	A	3	0	0	0	0
4	В	3	0	0	0	0
4	С	2	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	Н	7	0	0	0	0
4	I	13	0	0	0	0
4	J	10	0	0	0	0
4	K	4	0	0	0	0
4	L	2	0	0	0	0
4	M	3	0	0	0	0
4	N	3	0	0	0	0
All	All	19269	0	18822	243	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 6.

The worst 5 of 243 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
2:A:302:7SR:BR1	1:B:79:LEU:HD12	2.32	0.84	
1:F:111:ASN:HD21	1:F:140:LEU:HD12	1.43	0.83	
1:A:105:PHE:HB2	2:A:302:7SR:BR1	2.34	0.83	
1:E:213:THR:HG21	1:E:220:ILE:HD11	1.60	0.82	
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.66	0.77	

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	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
1	В	$164/221 \ (74\%)$	159 (97%)	5 (3%)	0	100	100
1	С	$162/221 \ (73\%)$	158 (98%)	4 (2%)	0	100	100
1	D	164/221 (74%)	158 (96%)	6 (4%)	0	100	100
1	E	165/221 (75%)	160 (97%)	5 (3%)	0	100	100
1	F	165/221 (75%)	161 (98%)	4 (2%)	0	100	100
1	G	164/221 (74%)	161 (98%)	3 (2%)	0	100	100
1	Н	176/221 (80%)	169 (96%)	7 (4%)	0	100	100
1	I	172/221 (78%)	167 (97%)	5 (3%)	0	100	100
1	J	172/221 (78%)	167 (97%)	5 (3%)	0	100	100
1	K	170/221 (77%)	164 (96%)	6 (4%)	0	100	100
1	L	173/221 (78%)	168 (97%)	5 (3%)	0	100	100
1	M	175/221 (79%)	170 (97%)	5 (3%)	0	100	100
1	N	175/221 (79%)	170 (97%)	5 (3%)	0	100	100
All	All	2361/3094 (76%)	2291 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 Outlier		Percentiles	
1	A	143/185~(77%)	143 (100%)	0	100	100
1	В	142/185~(77%)	140 (99%)	2 (1%)	67	78
1	С	135/185~(73%)	132 (98%)	3 (2%)	52	66
1	D	$137/185 \ (74\%)$	134 (98%)	3 (2%)	52	66
1	E	143/185~(77%)	137 (96%)	6 (4%)	30	40
1	F	145/185~(78%)	143 (99%)	2 (1%)	67	78
1	G	145/185~(78%)	141 (97%)	4 (3%)	43	56



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Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	Н	153/185 (83%)	153 (100%)	0	100	100	
1	I	149/185 (80%)	147 (99%)	2 (1%)	69	80	
1	J	147/185 (80%)	146 (99%)	1 (1%)	84	90	
1	K	142/185 (77%)	140 (99%)	2 (1%)	67	78	
1	L	152/185~(82%)	150 (99%)	2 (1%)	69	80	
1	M	145/185 (78%)	144 (99%)	1 (1%)	84	90	
1	N	149/185 (80%)	147 (99%)	2 (1%)	69	80	
All	All	2027/2590 (78%)	1997 (98%)	30 (2%)	65	77	

5 of 30 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	F	79	LEU
1	M	82	GLU
1	G	111	ASN
1	N	88	MET
1	K	141	ASN

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

Mol	Chain	Res	Type
1	С	107	GLN
1	I	107	GLN
1	L	107	GLN
1	L	168	HIS

#### 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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	В	ond leng	gths	В	ond ang	gles
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	7SR	N	301	-	40,42,42	3.31	13 (32%)	52,60,60	1.71	8 (15%)
2	7SR	A	302	-	40,42,42	3.33	11 (27%)	52,60,60	1.65	9 (17%)
2	7SR	G	301	-	40,42,42	3.28	8 (20%)	52,60,60	1.24	3 (5%)
2	7SR	L	301	-	40,42,42	3.23	9 (22%)	52,60,60	1.39	6 (11%)
2	7SR	I	301	-	40,42,42	3.25	8 (20%)	52,60,60	1.36	6 (11%)
2	7SR	В	301	-	40,42,42	3.09	12 (30%)	52,60,60	2.06	10 (19%)
2	7SR	D	301	-	40,42,42	3.15	9 (22%)	52,60,60	2.34	14 (26%)
2	7SR	A	301	-	40,42,42	3.28	8 (20%)	52,60,60	1.20	5 (9%)
2	7SR	D	302	-	40,42,42	3.29	11 (27%)	52,60,60	1.36	5 (9%)
2	7SR	I	302	-	40,42,42	3.04	16 (40%)	52,60,60	1.62	8 (15%)
2	7SR	Н	301	-	40,42,42	3.15	8 (20%)	52,60,60	1.30	8 (15%)
2	7SR	K	301	-	40,42,42	3.39	15 (37%)	52,60,60	1.82	11 (21%)
2	7SR	K	302	-	40,42,42	3.15	8 (20%)	52,60,60	1.28	7 (13%)
2	7SR	Е	301	-	40,42,42	3.29	9 (22%)	52,60,60	1.98	5 (9%)

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	7SR	N	301	-	-	0/19/52/52	0/5/5/5
2	7SR	A	302	-	-	4/19/52/52	0/5/5/5
2	7SR	G	301	-	-	7/19/52/52	0/5/5/5
2	7SR	L	301	-	-	1/19/52/52	0/5/5/5
2	7SR	I	301	-	-	0/19/52/52	0/5/5/5
2	7SR	В	301	-	-	2/19/52/52	0/5/5/5



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Mol	Type	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	7SR	D	301	-	-	5/19/52/52	0/5/5/5
2	7SR	A	301	-	-	3/19/52/52	0/5/5/5
2	7SR	D	302	-	-	5/19/52/52	0/5/5/5
2	7SR	I	302	-	-	1/19/52/52	0/5/5/5
2	7SR	Н	301	_	-	0/19/52/52	0/5/5/5
2	7SR	K	301	-	-	0/19/52/52	0/5/5/5
2	7SR	K	302	_	-	0/19/52/52	0/5/5/5
2	7SR	E	301	_	_	6/19/52/52	0/5/5/5

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
2	Ε	301	7SR	C6-N7	16.54	1.49	1.35
2	I	301	7SR	C6-N7	16.46	1.49	1.35
2	A	301	7SR	C6-N7	16.44	1.49	1.35
2	A	302	7SR	C6-N7	16.20	1.49	1.35
2	G	301	7SR	C6-N7	16.19	1.49	1.35

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	Ε	301	7SR	C35-N34-C2	-11.29	110.67	120.84
2	D	301	7SR	C35-N34-C2	-7.87	113.75	120.84
2	D	301	7SR	C38-C37-C36	-7.19	111.14	121.03
2	I	302	7SR	C20-N19-C18	6.60	126.78	115.69
2	В	301	7SR	C35-N34-C2	-6.32	115.14	120.84

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	7SR	C21-C20-N19-C31
2	D	302	7SR	C31-C8-C9-C46
2	Е	301	7SR	C11-C10-C9-C8
2	Е	301	7SR	N7-C8-C9-C10
2	Е	301	7SR	N7-C8-C9-C46

There are no ring outliers.

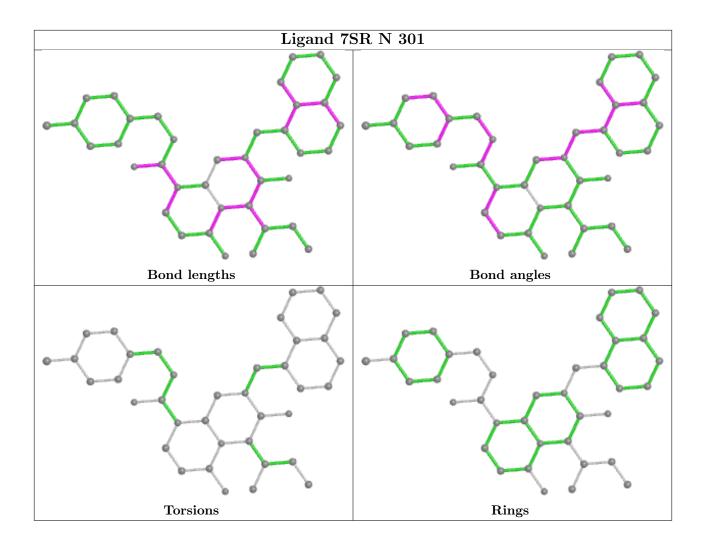
9 monomers are involved in 17 short contacts:



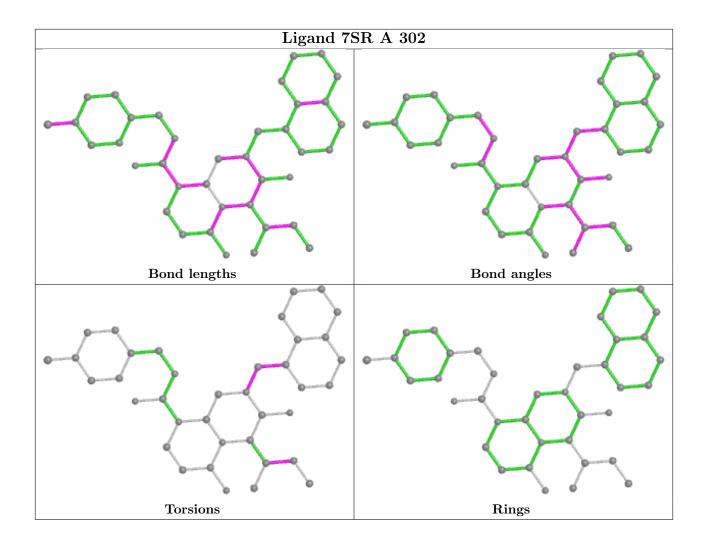
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	7SR	3	0
2	G	301	7SR	1	0
2	I	301	7SR	1	0
2	В	301	7SR	1	0
2	D	301	7SR	4	0
2	A	301	7SR	1	0
2	D	302	7SR	4	0
2	K	302	7SR	1	0
2	Е	301	7SR	1	0

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 then 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.

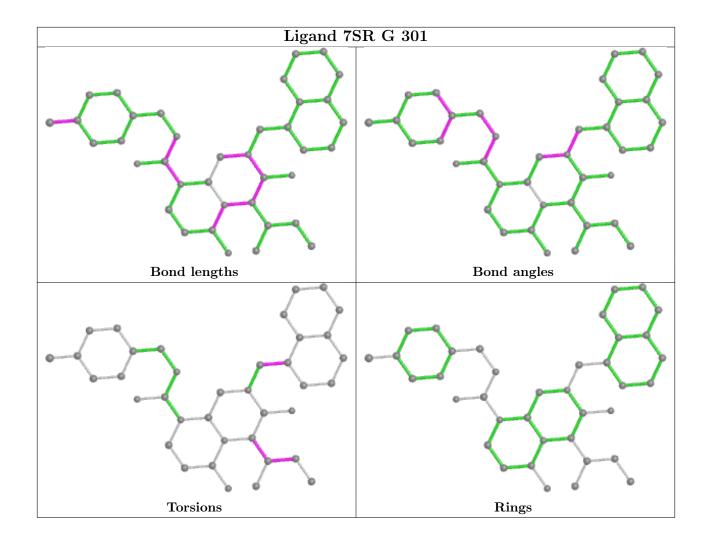




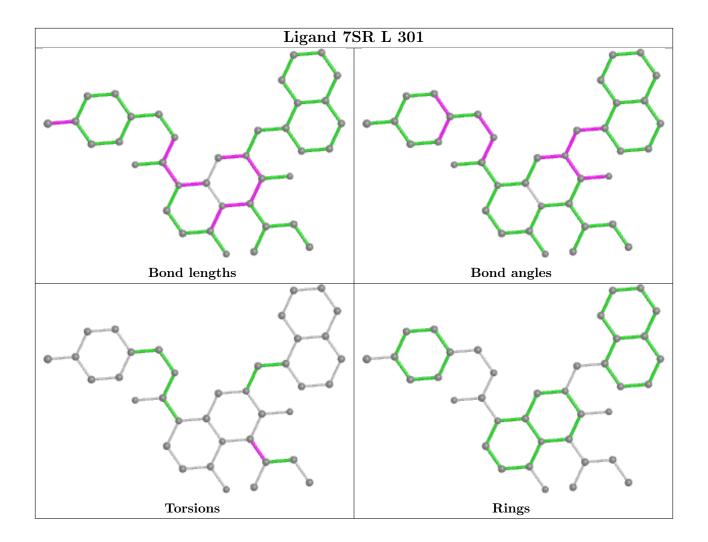




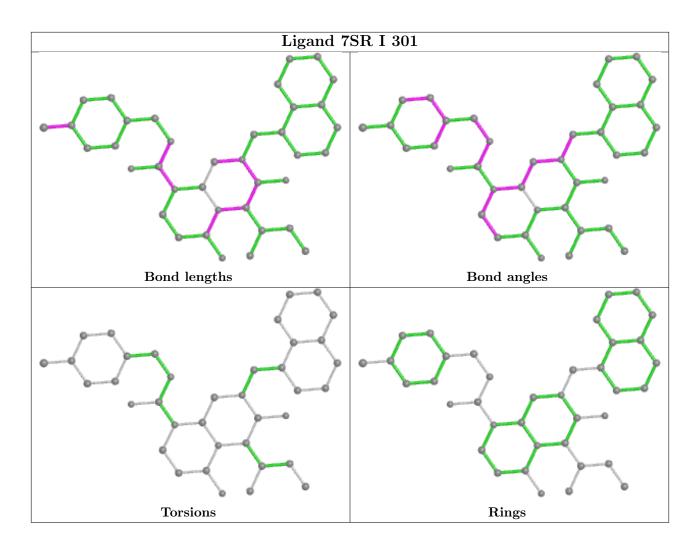




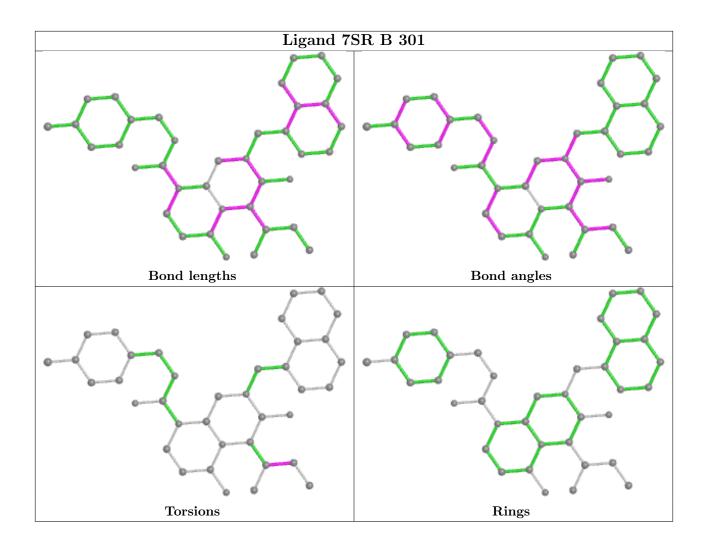




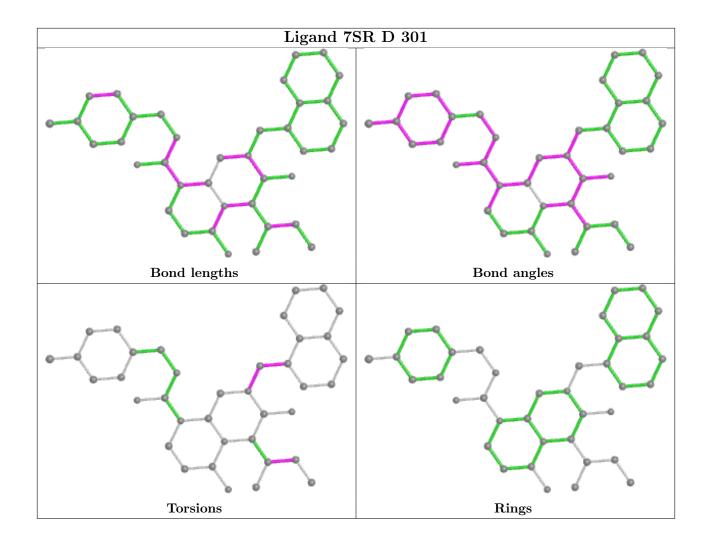




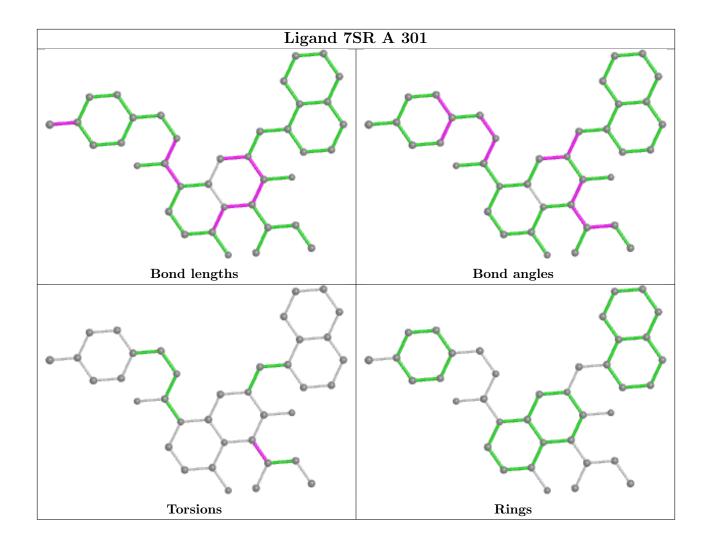




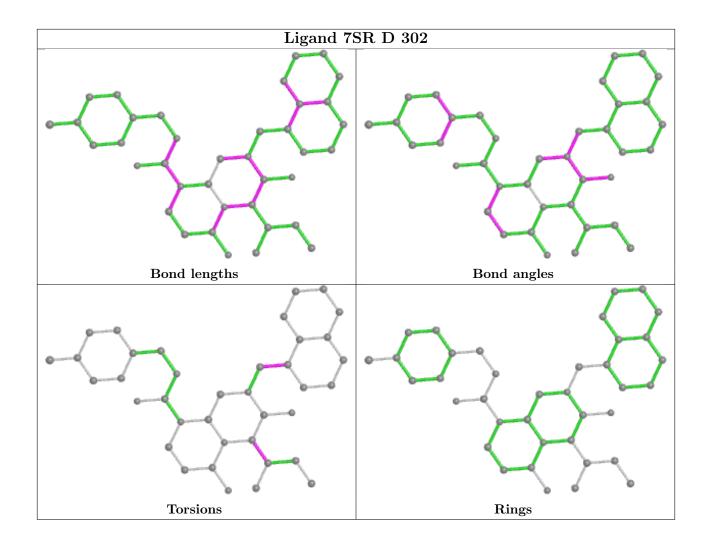




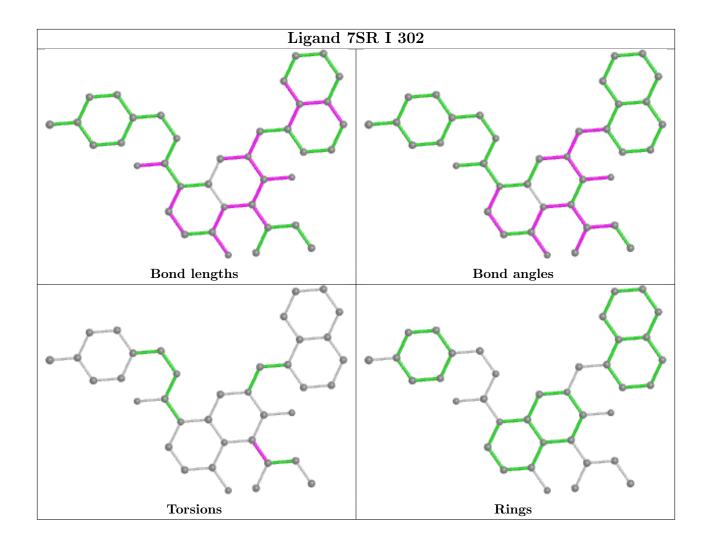




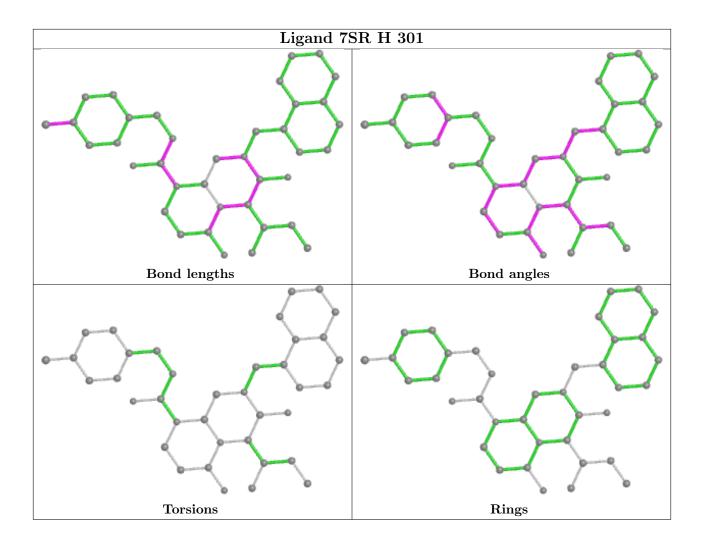




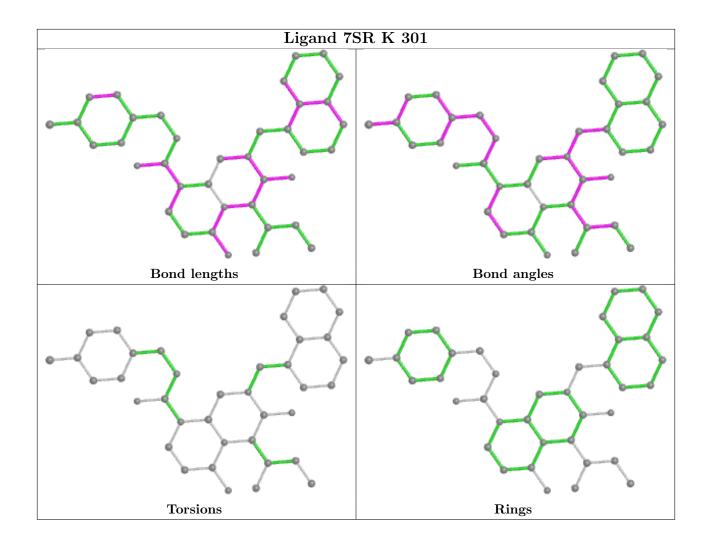




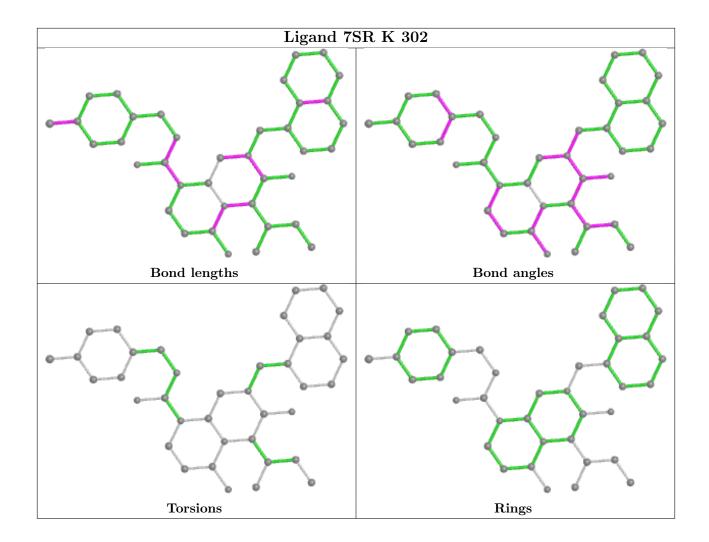




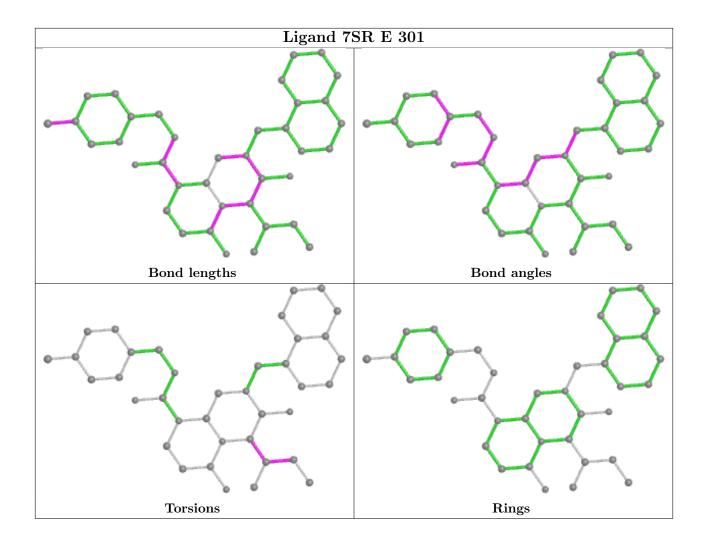












## 5.7 Other polymers (i)

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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	170/221 (76%)	0.11	5 (2%) 51 61	43, 58, 79, 99	0
1	В	170/221 (76%)	0.32	11 (6%) 18 23	49, 66, 85, 101	0
1	С	168/221 (76%)	0.39	10 (5%) 21 26	59, 82, 99, 111	0
1	D	170/221 (76%)	0.69	18 (10%) 6 9	63, 86, 101, 127	0
1	Е	171/221 (77%)	0.56	19 (11%) 5 7	59, 77, 94, 115	0
1	F	171/221 (77%)	0.27	8 (4%) 31 40	45, 64, 90, 111	0
1	G	170/221 (76%)	0.14	8 (4%) 31 40	42, 55, 82, 98	0
1	Н	180/221 (81%)	-0.10	3 (1%) 70 77	30, 47, 63, 84	0
1	I	178/221 (80%)	-0.29	2 (1%) 80 85	31, 41, 65, 87	0
1	J	178/221 (80%)	-0.22	2 (1%) 80 85	30, 40, 64, 79	0
1	K	176/221 (79%)	-0.09	3 (1%) 70 77	34, 45, 73, 89	0
1	L	179/221 (80%)	0.03	3 (1%) 70 77	42, 58, 80, 93	0
1	M	179/221 (80%)	0.38	15 (8%) 11 14	45, 68, 90, 106	0
1	N	179/221 (80%)	0.26	8 (4%) 33 42	42, 61, 79, 94	0
All	All	2439/3094 (78%)	0.17	115 (4%) 31 40	30, 61, 92, 127	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	TYR	5.9
1	M	66	THR	5.6
1	D	72	ALA	5.1
1	G	62	VAL	4.7
1	В	62	VAL	4.6



#### 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,  $95^{th}$  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.

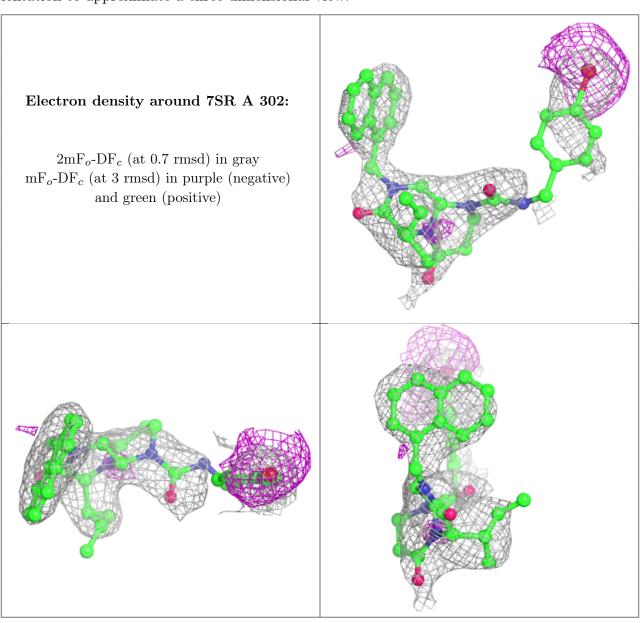
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	MG	N	302	1/1	0.74	0.22	77,77,77,77	0
3	MG	В	302	1/1	0.80	0.14	78,78,78,78	0
3	MG	D	303	1/1	0.83	0.31	79,79,79,79	0
3	MG	J	301	1/1	0.84	0.23	55,55,55,55	0
2	7SR	A	302	38/38	0.86	0.30	59,89,112,114	0
2	7SR	D	301	38/38	0.89	0.23	79,91,106,106	0
2	7SR	Ε	301	38/38	0.89	0.27	75,96,115,120	0
3	MG	L	302	1/1	0.90	0.17	70,70,70,70	0
3	MG	Ι	303	1/1	0.91	0.11	52,52,52,52	0
3	MG	F	301	1/1	0.91	0.15	74,74,74,74	0
2	7SR	В	301	38/38	0.92	0.17	84,94,99,107	0
3	MG	M	301	1/1	0.92	0.12	79,79,79,79	0
2	7SR	D	302	38/38	0.92	0.20	85,95,130,137	0
3	MG	С	301	1/1	0.93	0.08	98,98,98,98	0
2	7SR	G	301	38/38	0.93	0.16	63,78,102,116	0
3	MG	Ε	302	1/1	0.94	0.20	67,67,67,67	0
2	7SR	A	301	38/38	0.95	0.14	58,68,84,97	0
2	7SR	L	301	38/38	0.95	0.14	57,63,71,81	0
3	MG	A	303	1/1	0.96	0.31	65,65,65,65	0
2	7SR	Н	301	38/38	0.96	0.13	44,51,64,64	0
2	7SR	N	301	38/38	0.96	0.12	56,65,70,74	0
3	MG	G	302	1/1	0.96	0.21	60,60,60,60	0
3	MG	Н	302	1/1	0.96	0.13	42,42,42,42	0
2	7SR	K	302	38/38	0.97	0.12	28,44,57,63	0
2	7SR	I	302	38/38	0.98	0.09	37,46,60,69	0
2	7SR	K	301	38/38	0.98	0.10	41,46,55,61	0
2	7SR	I	301	38/38	0.98	0.12	30,40,49,58	0



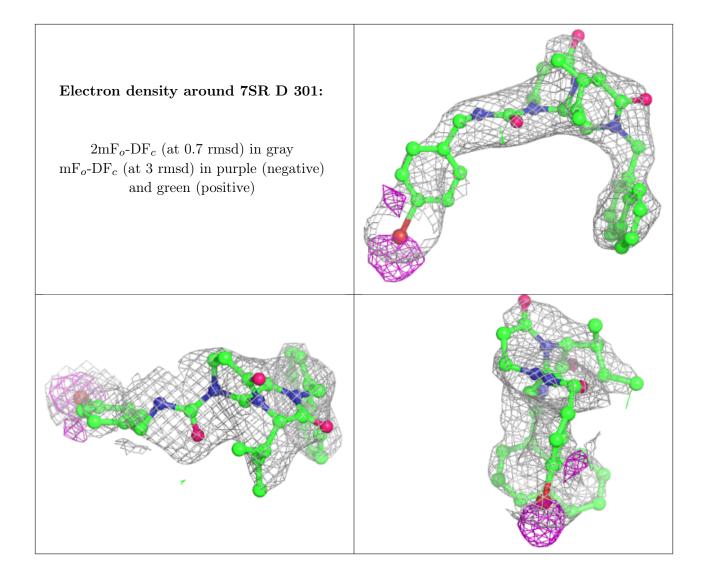
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	MG	K	303	1/1	0.99	0.07	45,45,45,45	0

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.



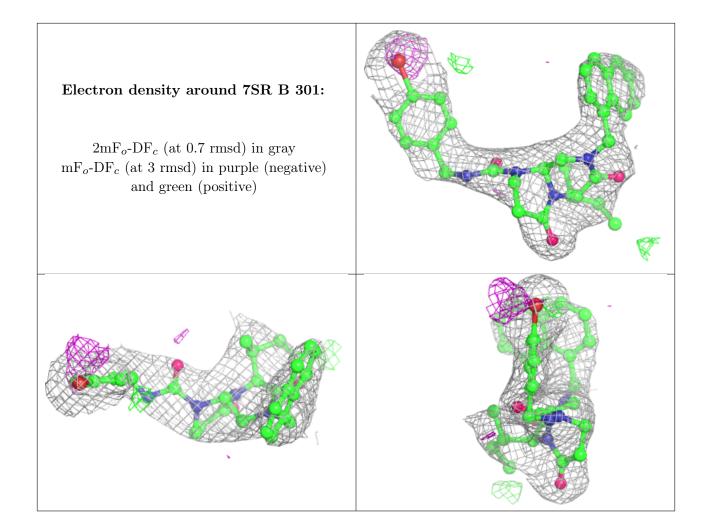






## Electron density around 7SR E 301: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

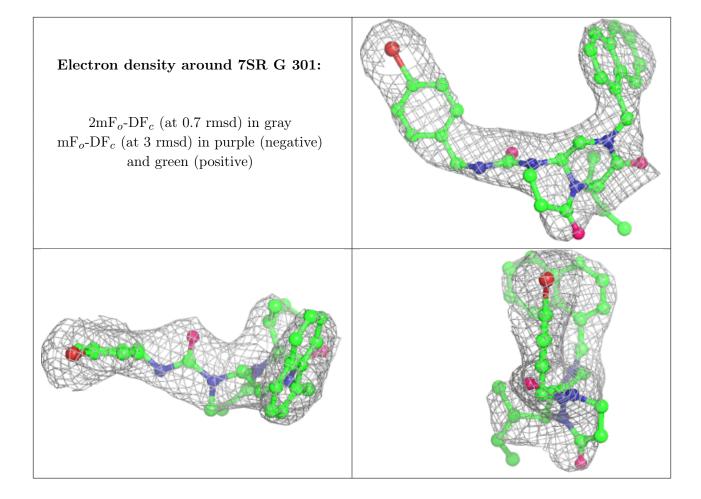




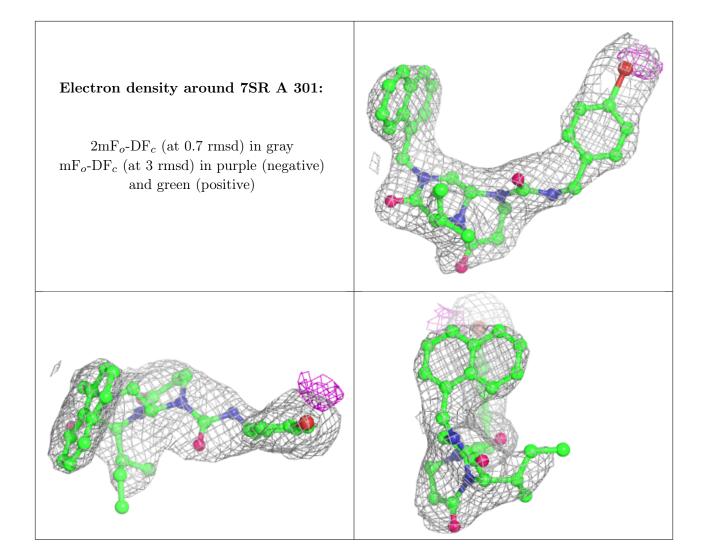


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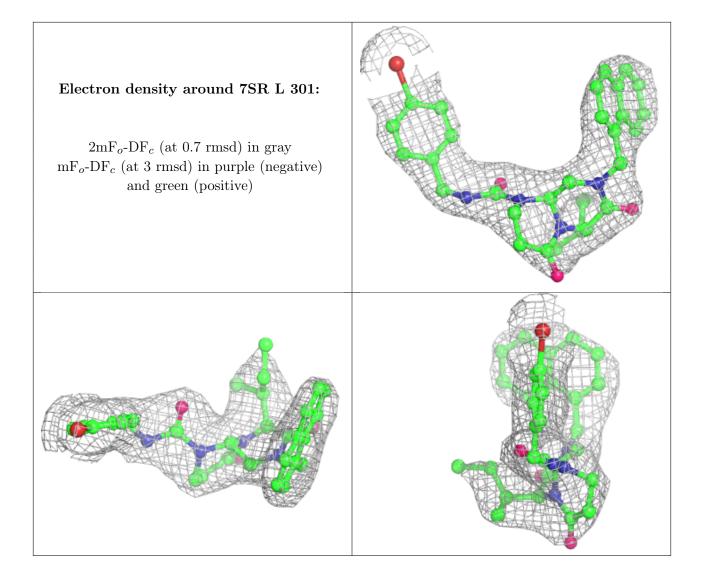




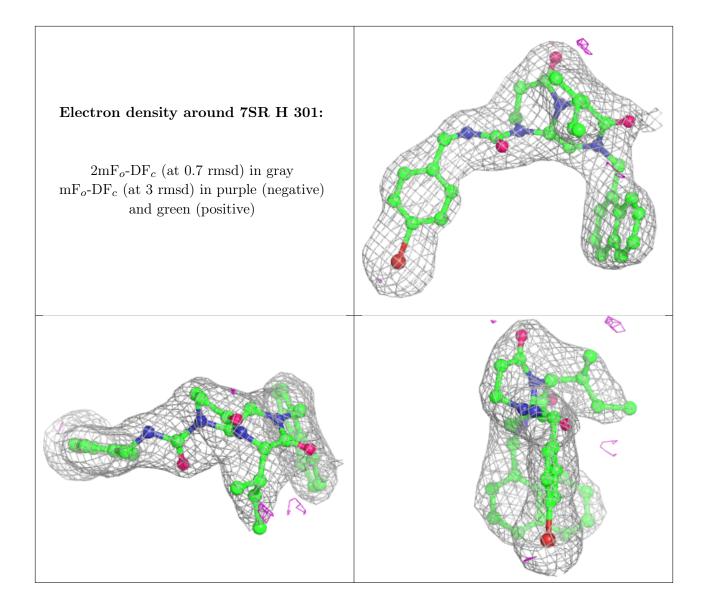




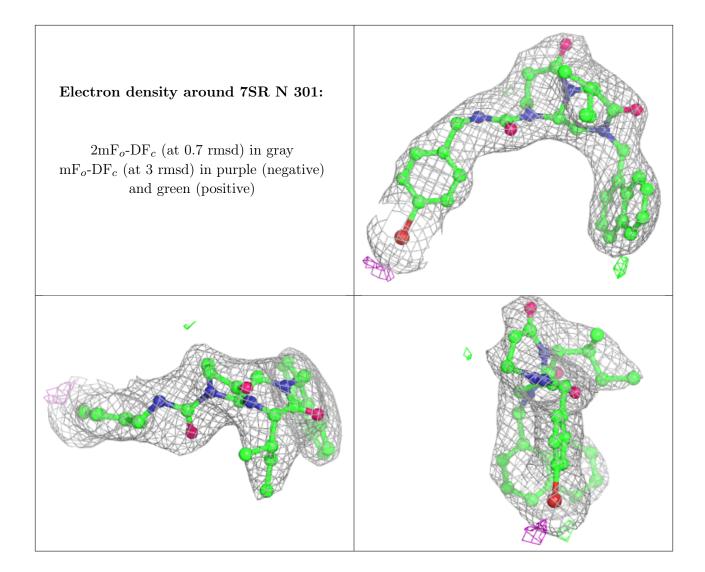








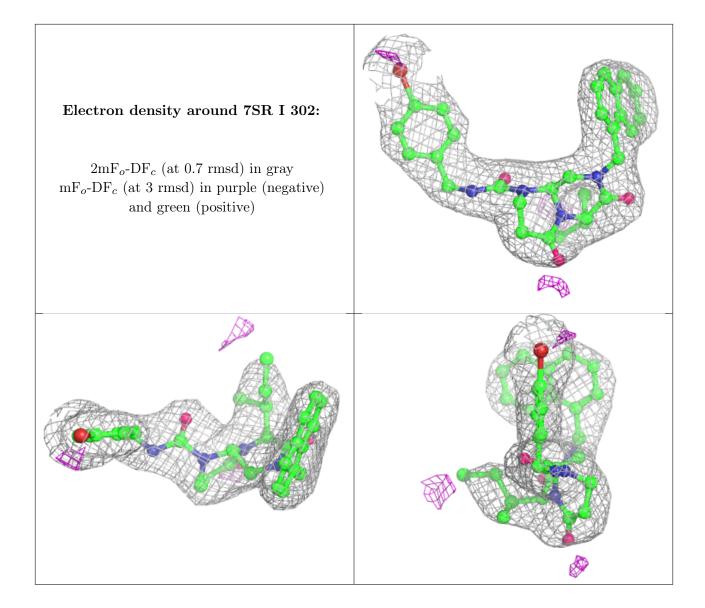




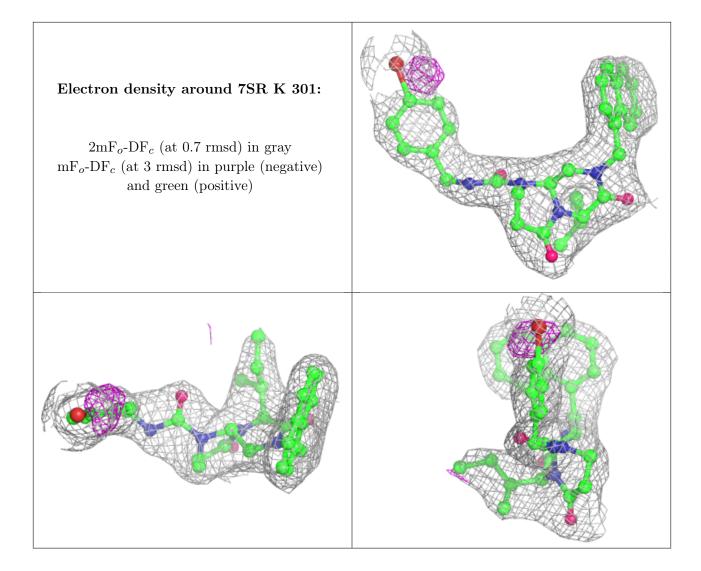


## Electron density around 7SR K 302: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)

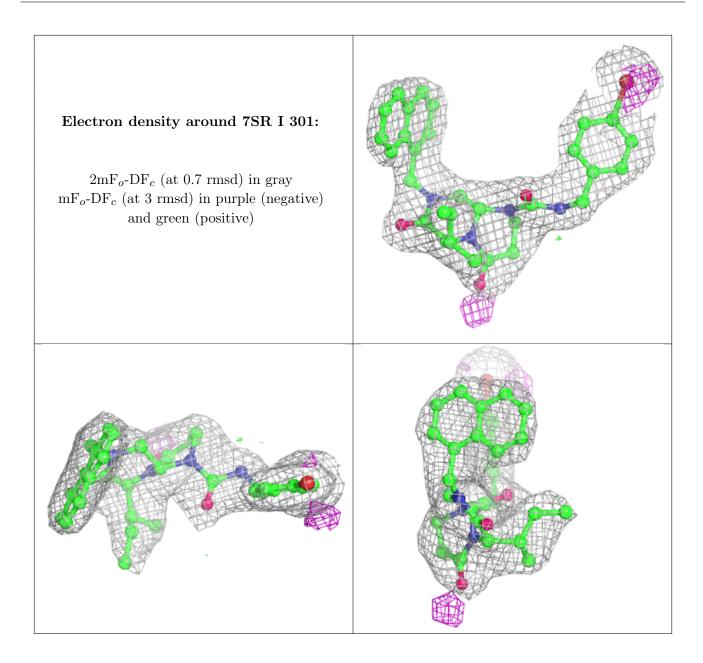












## 6.5 Other polymers (i)

There are no such residues in this entry.

