



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 12:13 PM JST

PDB ID : 7VDR  
Title : The structure of cyclin-dependent kinase 5 (CDK5) in complex with p25 and Compound 13  
Authors : Malojcic, G.; Clugston, S.L.; Daniels, M.; Harmange, J.C.; Ledeborer, M.  
Deposited on : 2021-09-07  
Resolution : 2.55 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](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 : 2.27  
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) : 2.27

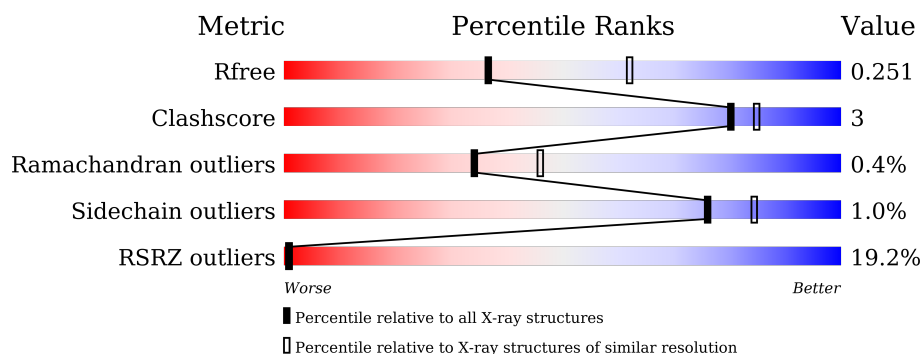
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	292	<div> <div>6%</div> <div>93%</div> <div>7%</div> </div>
1	B	292	<div> <div>17%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
2	C	209	<div> <div>%</div> <div>65%</div> <div>6%</div> <div>29%</div> </div>
2	D	209	<div> <div>44%</div> <div>58%</div> <div>7%</div> <div>35%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	303	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7028 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 Cyclin-dependent-like kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2330	1495	400	424	11			
1	B	275	Total	C	N	O	S	0	0	0
			2217	1428	384	395	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q00535
B	1	SER	-	expression tag	UNP Q00535

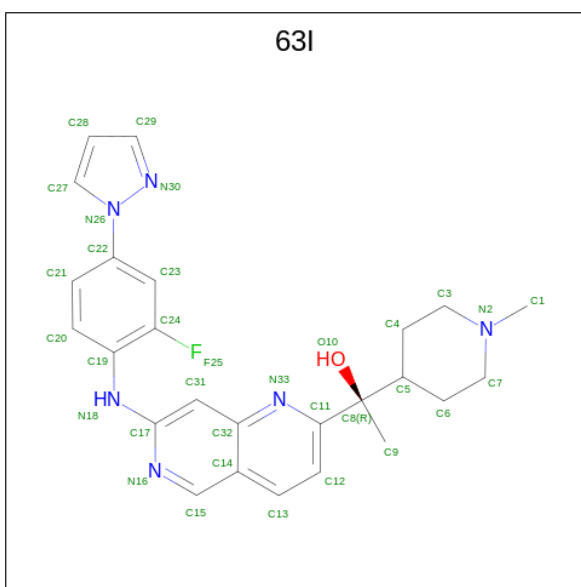
- Molecule 2 is a protein called Cyclin-dependent kinase 5 activator 1, p25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	148	Total	C	N	O	S	0	0	0
			1196	768	197	220	11			
2	D	136	Total	C	N	O	S	0	0	0
			1104	711	179	204	10			

There are 2 discrepancies between the modelled and reference sequences:

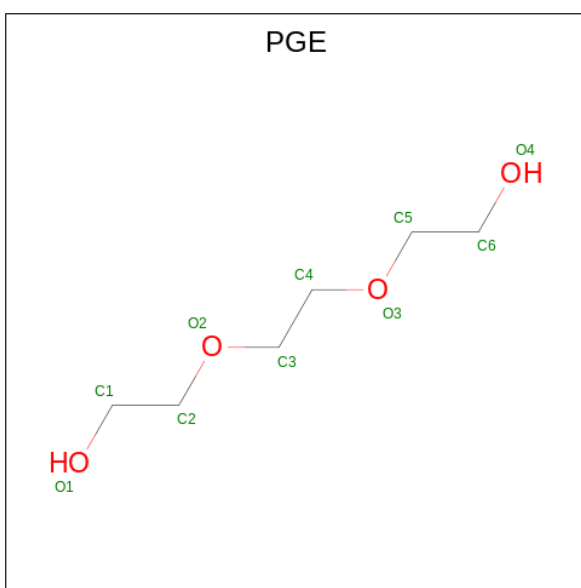
Chain	Residue	Modelled	Actual	Comment	Reference
C	99	MET	-	initiating methionine	UNP Q15078
D	99	MET	-	initiating methionine	UNP Q15078

- Molecule 3 is (1R)-1-[7-[(2-fluoranyl-4-pyrazol-1-yl-phenyl)amino]-1,6-naphthyridin-2-yl]-1-(1-methylpiperidin-4-yl)ethanol (three-letter code: 63I) (formula: C<sub>25</sub>H<sub>27</sub>FN<sub>6</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			33	25	1	6	1		
3	B	1	Total	C	F	N	O	0	0
			33	25	1	6	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

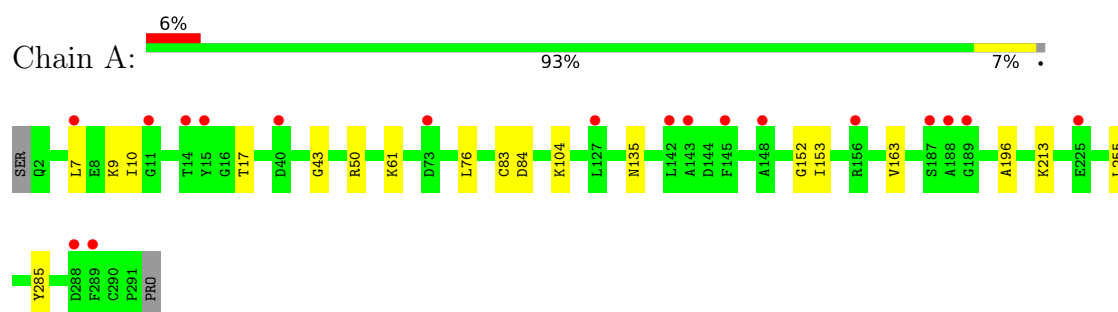
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total	O	0	0
			41	41		
6	B	15	Total	O	0	0
			15	15		
6	C	13	Total	O	0	0
			13	13		

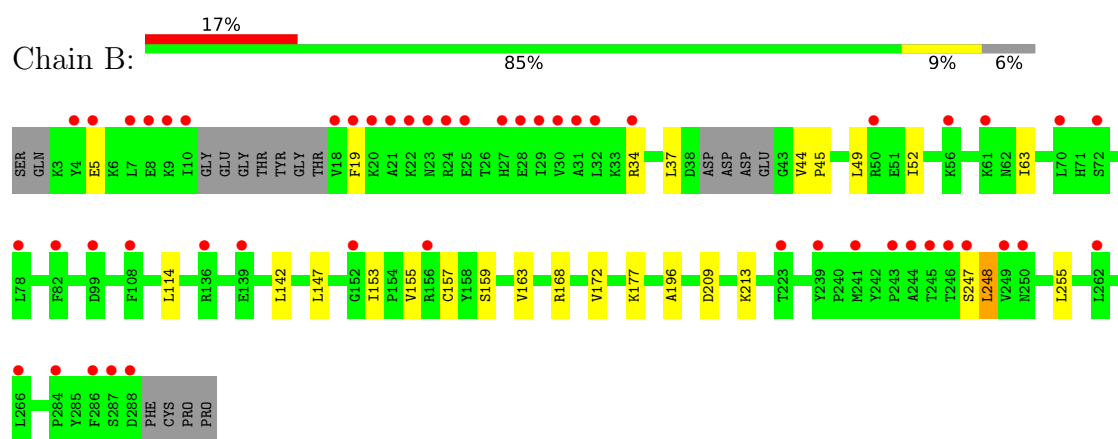
### 3 Residue-property plots [i](#)

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.

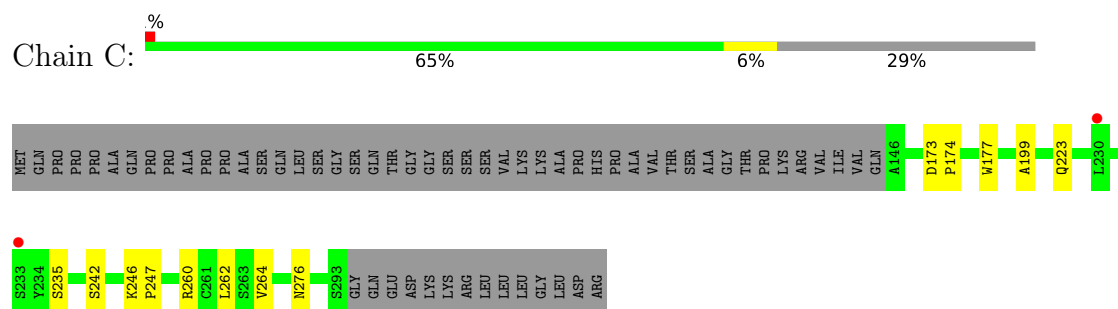
- Molecule 1: Cyclin-dependent-like kinase 5



- Molecule 1: Cyclin-dependent-like kinase 5



- Molecule 2: Cyclin-dependent kinase 5 activator 1, p25



- Molecule 2: Cyclin-dependent kinase 5 activator 1, p25

[illegible]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.83Å 117.83Å 154.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.65 – 2.55 29.65 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.65-2.55) 100.0 (29.65-2.55)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.219 , 0.256 0.220 , 0.251	Depositor DCC
$R_{free}$ test set	1980 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: EDO, PGE, 63I

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	0.63	0/2385	0.77	0/3229
1	B	0.65	0/2267	0.75	0/3065
2	C	0.65	0/1224	0.73	0/1660
2	D	0.67	0/1129	0.70	0/1530
All	All	0.65	0/7005	0.75	0/9484

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 [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	2330	0	2344	12	0
1	B	2217	0	2257	16	0
2	C	1196	0	1185	9	0
2	D	1104	0	1088	9	0
3	A	33	0	0	1	0
3	B	33	0	0	0	0
4	A	10	0	14	0	0
5	A	32	0	48	0	0
5	C	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	41	0	0	1	0
6	B	15	0	0	0	0
6	C	13	0	0	0	0
All	All	7028	0	6942	37	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 3.

All (37) 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:83:CYS:HA	1:A:135:ASN:HD21	1.45	0.81
1:B:247:SER:O	1:B:248:LEU:HB2	1.91	0.70
1:B:19:PHE:HE1	1:B:34:ARG:HD3	1.63	0.63
1:B:157:CYS:HB2	1:B:177:LYS:HB3	1.85	0.58
2:D:204:LEU:HD12	2:D:229:CYS:SG	2.45	0.57
1:B:37:LEU:HD23	2:D:258:TRP:CD1	2.42	0.54
1:B:44:VAL:N	1:B:45:PRO:HD2	2.23	0.53
1:B:49:LEU:HA	1:B:52:ILE:HD12	1.92	0.52
1:A:83:CYS:HA	1:A:135:ASN:ND2	2.20	0.52
1:A:43:GLY:O	2:C:242:SER:HB2	2.11	0.51
1:B:63:ILE:HD13	1:B:142:LEU:HB3	1.96	0.48
2:C:246:LYS:HB3	2:C:247:PRO:HD3	1.96	0.47
1:A:50:ARG:NH1	2:C:235:SER:O	2.47	0.47
1:A:152:GLY:HA3	2:C:276:ASN:O	2.15	0.47
1:B:168:ARG:HD3	1:B:172:VAL:HG12	1.97	0.46
1:B:159:SER:HB2	2:D:239:ASN:O	2.16	0.46
2:D:246:LYS:HB3	2:D:247:PRO:HD3	1.98	0.46
1:B:196:ALA:HB1	1:B:255:LEU:HG	1.97	0.46
1:B:209:ASP:OD1	1:B:213:LYS:HE2	2.15	0.45
2:C:177:TRP:CD2	2:C:223:GLN:HG3	2.52	0.44
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.89	0.44
1:B:153:ILE:O	1:B:155:VAL:HG23	2.18	0.43
1:B:49:LEU:HD11	2:D:235:SER:CB	2.48	0.42
2:D:190:TRP:CD1	2:D:244:PRO:HG3	2.55	0.42
1:A:84:ASP:H	1:A:135:ASN:HD22	1.68	0.42
2:D:207:LEU:HB2	2:D:229:CYS:SG	2.59	0.42
2:D:260:ARG:O	2:D:264:VAL:HG23	2.19	0.42
1:B:49:LEU:HB2	2:D:265:ILE:HD11	2.01	0.42
1:B:19:PHE:CE1	1:B:34:ARG:HD3	2.49	0.41
1:A:76:LEU:HD11	2:C:262:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG23	3:A:301:63I:C23	2.51	0.41
1:A:196:ALA:HB1	1:A:255:LEU:HG	2.02	0.41
1:A:213:LYS:NZ	6:A:403:HOH:O	2.54	0.41
2:C:260:ARG:O	2:C:264:VAL:HG23	2.21	0.41
1:A:153:ILE:HG21	2:C:199:ALA:HB1	2.02	0.41
1:A:104:LYS:NZ	1:A:285:TYR:O	2.41	0.40
2:C:173:ASP:HB2	2:C:174:PRO:HD3	2.02	0.40

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	288/292 (99%)	276 (96%)	11 (4%)	1 (0%)	41	51
1	B	269/292 (92%)	253 (94%)	14 (5%)	2 (1%)	22	30
2	C	146/209 (70%)	146 (100%)	0	0	100	100
2	D	130/209 (62%)	126 (97%)	4 (3%)	0	100	100
All	All	833/1002 (83%)	801 (96%)	29 (4%)	3 (0%)	34	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	VAL
1	B	163	VAL
1	B	248	LEU

### 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	258/260 (99%)	254 (98%)	4 (2%)	62	77
1	B	246/260 (95%)	244 (99%)	2 (1%)	81	88
2	C	138/187 (74%)	138 (100%)	0	100	100
2	D	128/187 (68%)	126 (98%)	2 (2%)	62	77
All	All	770/894 (86%)	762 (99%)	8 (1%)	76	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	LYS
1	A	17	THR
1	A	61	LYS
1	B	5	GLU
1	B	147	LEU
2	D	170	SER
2	D	259	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
2	D	188	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	$\# Z  > 2$
5	EDO	A	306	-	3,3,3	0.09	0	2,2,2	0.07	0
5	EDO	A	305	-	3,3,3	0.04	0	2,2,2	0.15	0
5	EDO	A	308	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	A	309	-	3,3,3	0.15	0	2,2,2	0.37	0
5	EDO	C	401	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	A	307	-	3,3,3	0.08	0	2,2,2	0.14	0
3	63I	A	301	-	34,37,37	0.67	0	47,54,54	2.68	11 (23%)
5	EDO	A	310	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	A	303	-	3,3,3	0.11	0	2,2,2	0.27	0
5	EDO	A	304	-	3,3,3	0.06	0	2,2,2	0.18	0
3	63I	B	301	-	34,37,37	0.77	0	47,54,54	2.60	11 (23%)
4	PGE	A	302	-	9,9,9	0.23	0	8,8,8	0.10	0

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	EDO	A	306	-	-	1/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	A	308	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	C	401	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
3	63I	A	301	-	-	5/19/30/30	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	310	-	-	0/1/1/1	-
5	EDO	A	303	-	-	1/1/1/1	-
5	EDO	A	304	-	-	1/1/1/1	-
3	63I	B	301	-	-	5/19/30/30	0/5/5/5
4	PGE	A	302	-	-	4/7/7/7	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	63I	C27-N26-N30	-8.16	106.43	111.94
3	B	301	63I	C22-N26-N30	7.67	125.60	118.80
3	B	301	63I	C27-N26-N30	-7.56	106.84	111.94
3	A	301	63I	C22-N26-N30	7.55	125.50	118.80
3	A	301	63I	C29-N30-N26	7.29	109.01	103.70
3	B	301	63I	C29-N30-N26	7.24	108.97	103.70
3	A	301	63I	C11-N33-C32	7.08	122.64	117.36
3	B	301	63I	C11-N33-C32	6.42	122.15	117.36
3	A	301	63I	C15-N16-C17	5.04	122.91	117.81
3	B	301	63I	C15-N16-C17	4.87	122.74	117.81
3	A	301	63I	C31-C32-N33	3.04	123.34	118.72
3	B	301	63I	C3-N2-C7	2.98	113.69	109.52
3	B	301	63I	C31-C32-N33	2.86	123.06	118.72
3	B	301	63I	C21-C22-N26	2.82	121.62	119.15
3	A	301	63I	C9-C8-C5	-2.82	108.70	112.46
3	B	301	63I	C23-C24-C19	-2.78	120.85	123.50
3	A	301	63I	C21-C22-C23	-2.49	118.80	121.74
3	B	301	63I	C21-C22-C23	-2.48	118.80	121.74
3	A	301	63I	C14-C32-N33	-2.26	118.90	122.26
3	A	301	63I	C28-C27-N26	2.16	108.72	107.08
3	B	301	63I	C12-C11-C8	-2.10	118.81	122.14
3	A	301	63I	C21-C22-N26	2.04	120.94	119.15

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	63I	C12-C11-C8-C5
3	B	301	63I	C12-C11-C8-C5
4	A	302	PGE	O1-C1-C2-O2
5	A	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	304	EDO	O1-C1-C2-O2
5	A	306	EDO	O1-C1-C2-O2
3	B	301	63I	C12-C11-C8-C9
4	A	302	PGE	O3-C5-C6-O4
3	A	301	63I	C12-C11-C8-C9
5	A	307	EDO	O1-C1-C2-O2
3	B	301	63I	C12-C11-C8-O10
4	A	302	PGE	C1-C2-O2-C3
3	B	301	63I	C21-C22-N26-C27
3	B	301	63I	C23-C22-N26-C27
3	A	301	63I	C23-C22-N26-C27
5	A	308	EDO	O1-C1-C2-O2
5	C	401	EDO	O1-C1-C2-O2
3	A	301	63I	C12-C11-C8-O10
3	A	301	63I	C21-C22-N26-C27
4	A	302	PGE	O2-C3-C4-O3

There are no ring outliers.

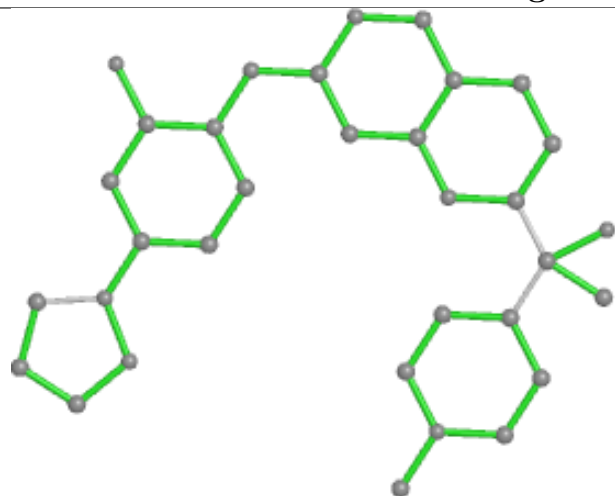
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	63I	1	0

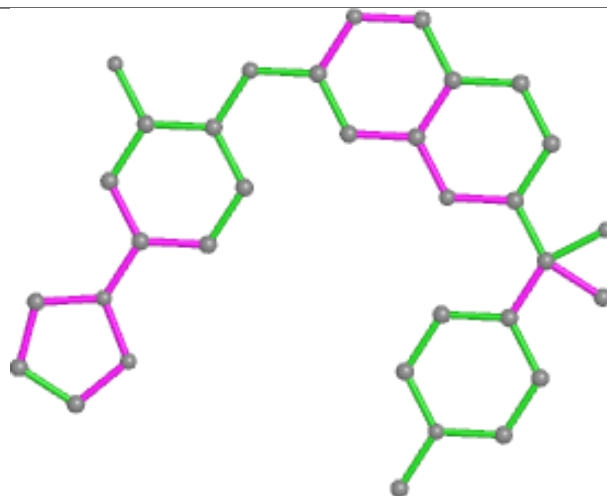
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



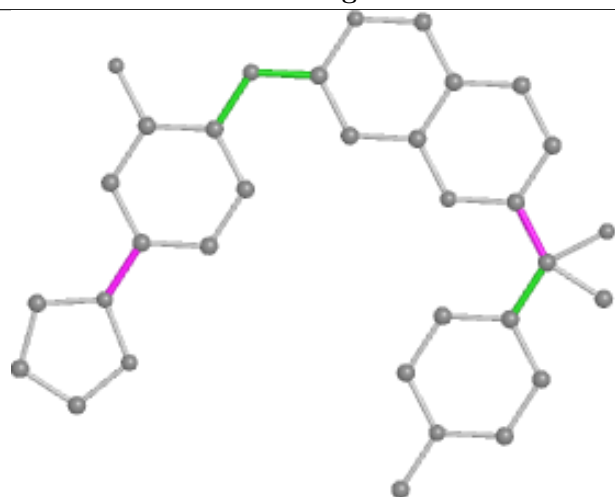
## Ligand 63I A 301



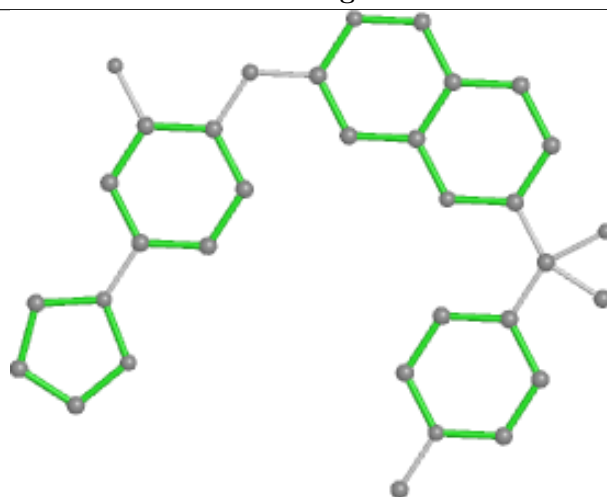
Bond lengths



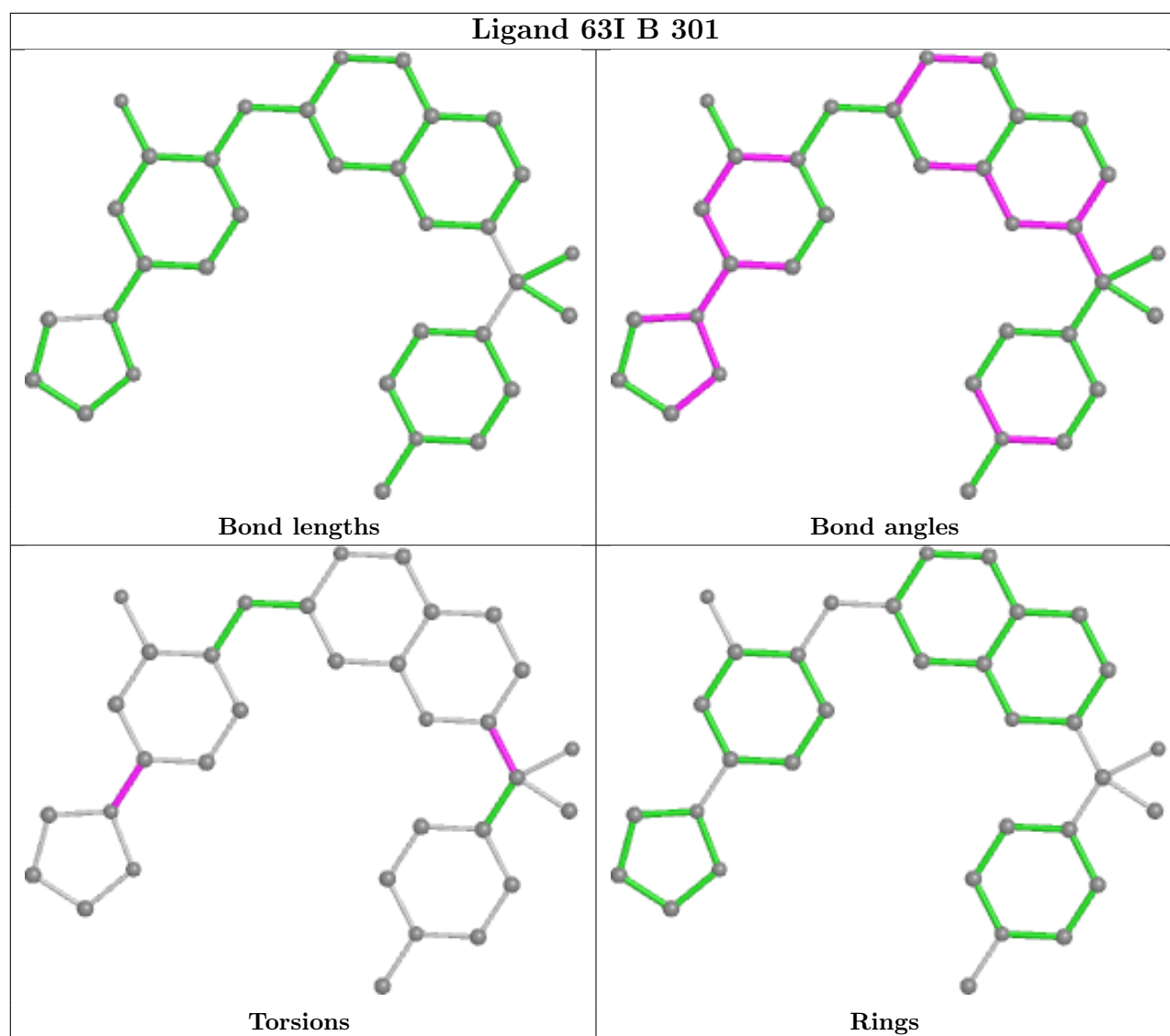
Bond angles



Torsions



Rings



## 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, 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	290/292 (99%)	0.44	18 (6%)	20 24	39, 54, 96, 139	0
1	B	275/292 (94%)	1.09	50 (18%)	1 1	52, 83, 136, 175	0
2	C	148/209 (70%)	0.28	2 (1%)	75 81	40, 53, 78, 87	0
2	D	136/209 (65%)	3.24	93 (68%)	0 0	117, 155, 173, 182	0
All	All	849/1002 (84%)	1.07	163 (19%)	1 1	39, 70, 164, 182	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	164	TYR	9.2
2	D	291	ASN	8.8
2	D	226	LEU	8.8
2	D	222	LEU	8.4
1	B	245	THR	8.3
2	D	216	VAL	7.7
2	D	175	VAL	7.5
2	D	151	LEU	7.0
1	B	247	SER	7.0
2	D	280	HIS	6.8
2	D	168	HIS	6.7
1	B	22	LYS	6.6
2	D	252	SER	6.6
1	A	14	THR	6.5
2	D	177	TRP	6.4
2	D	187	LEU	6.3
2	D	196	ILE	6.1
1	A	40	ASP	6.1
2	D	292	GLU	6.1
2	D	205	TYR	6.0
1	B	29	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
2	D	220	HIS	5.9
1	B	156	ARG	5.8
2	D	283	THR	5.8
2	D	163	CYS	5.8
2	D	229	CYS	5.6
2	D	217	GLY	5.5
2	D	166	LEU	5.5
2	D	285	VAL	5.5
1	B	246	THR	5.4
1	B	19	PHE	5.4
2	D	224	ALA	5.4
2	D	219	ASP	5.2
2	D	203	PHE	5.2
2	D	225	VAL	5.2
1	A	15	TYR	5.1
2	D	153	ARG	5.0
2	D	189	GLY	4.9
2	D	279	PRO	4.9
2	D	169	LEU	4.8
2	D	253	CYS	4.7
2	D	207	LEU	4.7
1	B	9	LYS	4.6
2	D	167	LYS	4.6
2	D	155	LEU	4.6
2	D	152	LEU	4.6
2	D	227	LEU	4.6
1	B	244	ALA	4.5
1	B	21	ALA	4.5
2	D	249	LEU	4.5
2	D	150	GLU	4.5
2	D	192	ASP	4.5
1	B	10	ILE	4.4
2	D	209	ARG	4.4
2	D	284	GLN	4.4
1	B	250	ASN	4.4
2	D	250	VAL	4.4
2	D	183	ARG	4.2
2	D	248	PHE	4.0
2	D	176	LEU	3.9
2	D	231	TYR	3.9
2	D	165	ARG	3.9
2	D	282	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	202	VAL	3.8
1	B	5	GLU	3.8
2	D	290	LYS	3.8
2	D	278	ASP	3.8
1	B	30	VAL	3.7
2	D	178	LEU	3.7
1	B	4	TYR	3.6
2	D	218	SER	3.6
2	D	172	THR	3.6
1	B	27	HIS	3.6
2	D	235	SER	3.5
2	D	154	CYS	3.5
1	B	70	LEU	3.5
1	B	7	LEU	3.5
1	B	32	LEU	3.5
1	B	72	SER	3.4
2	D	246	LYS	3.4
1	B	287	SER	3.4
2	D	274	GLN	3.4
2	D	281	TYR	3.3
1	B	18	VAL	3.3
2	D	190	TRP	3.3
2	D	244	PRO	3.2
2	D	259	ASP	3.2
2	D	171	PRO	3.2
2	D	186	LEU	3.2
1	B	20	LYS	3.0
2	D	287	SER	3.0
1	B	152	GLY	3.0
1	A	156	ARG	3.0
1	B	82	PHE	3.0
1	B	288	ASP	3.0
1	A	11	GLY	3.0
2	D	170	SER	2.9
1	A	127	LEU	2.9
1	B	284	PRO	2.9
2	D	230	LEU	2.9
1	B	24	ARG	2.9
1	B	25	GLU	2.9
2	D	193	GLN	2.8
1	B	50	ARG	2.8
1	B	136	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	234	TYR	2.8
2	D	258	TRP	2.7
2	D	173	ASP	2.7
2	D	228	THR	2.7
2	D	271	LYS	2.7
2	D	288	ASP	2.7
2	D	263	SER	2.6
1	B	139	GLU	2.6
1	A	148	ALA	2.6
1	B	286	PHE	2.6
2	D	215	GLU	2.6
1	B	108	PHE	2.6
1	A	73	ASP	2.6
2	D	293	SER	2.5
2	D	236	TYR	2.5
1	A	143	ALA	2.5
2	D	199	ALA	2.5
1	A	289	PHE	2.5
1	B	8	GLU	2.5
2	D	254	LYS	2.5
1	A	288	ASP	2.5
1	B	61	LYS	2.4
2	D	179	ARG	2.4
1	A	7	LEU	2.4
2	D	206	MET	2.4
1	B	249	VAL	2.4
2	D	267	LEU	2.4
2	D	198	PRO	2.3
1	B	78	LEU	2.3
1	B	243	PRO	2.3
1	B	241	MET	2.3
2	D	233	SER	2.3
1	A	145	PHE	2.3
2	D	256	ALA	2.3
1	B	23	ASN	2.3
2	D	200	ASN	2.2
1	B	99	ASP	2.2
1	A	225	GLU	2.2
1	B	223	THR	2.2
1	A	188	ALA	2.2
1	B	239	TYR	2.2
1	B	262	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	277	ALA	2.2
2	C	230	LEU	2.2
1	B	266	LEU	2.1
1	A	187	SER	2.1
2	D	191	GLN	2.1
2	D	242	SER	2.1
1	B	34	ARG	2.1
1	A	189	GLY	2.1
1	B	56	LYS	2.1
2	D	270	SER	2.1
1	B	31	ALA	2.1
2	D	241	ILE	2.0
1	A	142	LEU	2.0
1	B	28	GLU	2.0
2	C	233	SER	2.0
2	D	210	ASP	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 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<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(Å <sup>2</sup> )	Q<0.9
5	EDO	A	309	4/4	0.69	0.37	65,73,74,74	0
5	EDO	A	304	4/4	0.74	0.32	87,89,90,91	0
5	EDO	A	310	4/4	0.74	0.29	92,93,94,94	0
4	PGE	A	302	10/10	0.75	0.24	79,97,106,107	0
5	EDO	A	303	4/4	0.79	0.44	74,76,78,79	0
5	EDO	A	308	4/4	0.80	0.23	81,83,84,87	0
5	EDO	A	305	4/4	0.83	0.29	83,86,87,90	0

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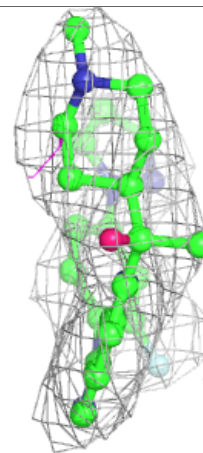
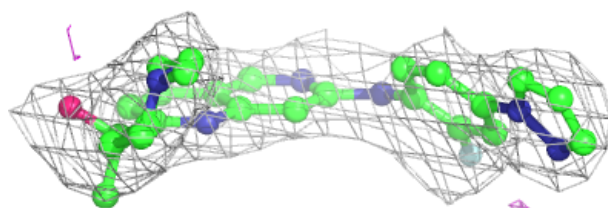
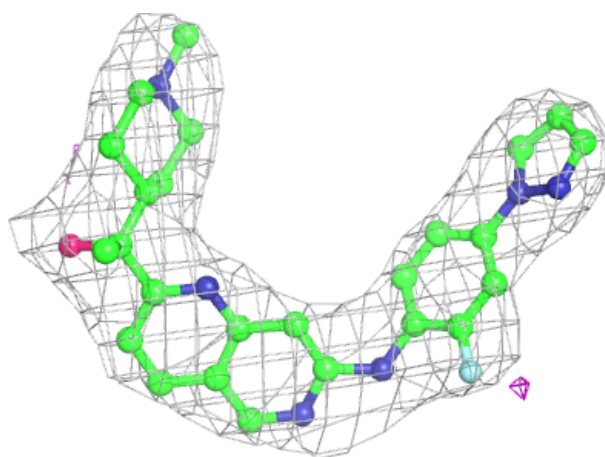
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	401	4/4	0.88	0.33	70,74,76,79	0
3	63I	B	301	33/33	0.92	0.18	68,85,95,95	0
5	EDO	A	306	4/4	0.93	0.25	70,71,71,71	0
3	63I	A	301	33/33	0.95	0.16	41,45,59,62	0
5	EDO	A	307	4/4	0.96	0.24	78,83,86,87	0

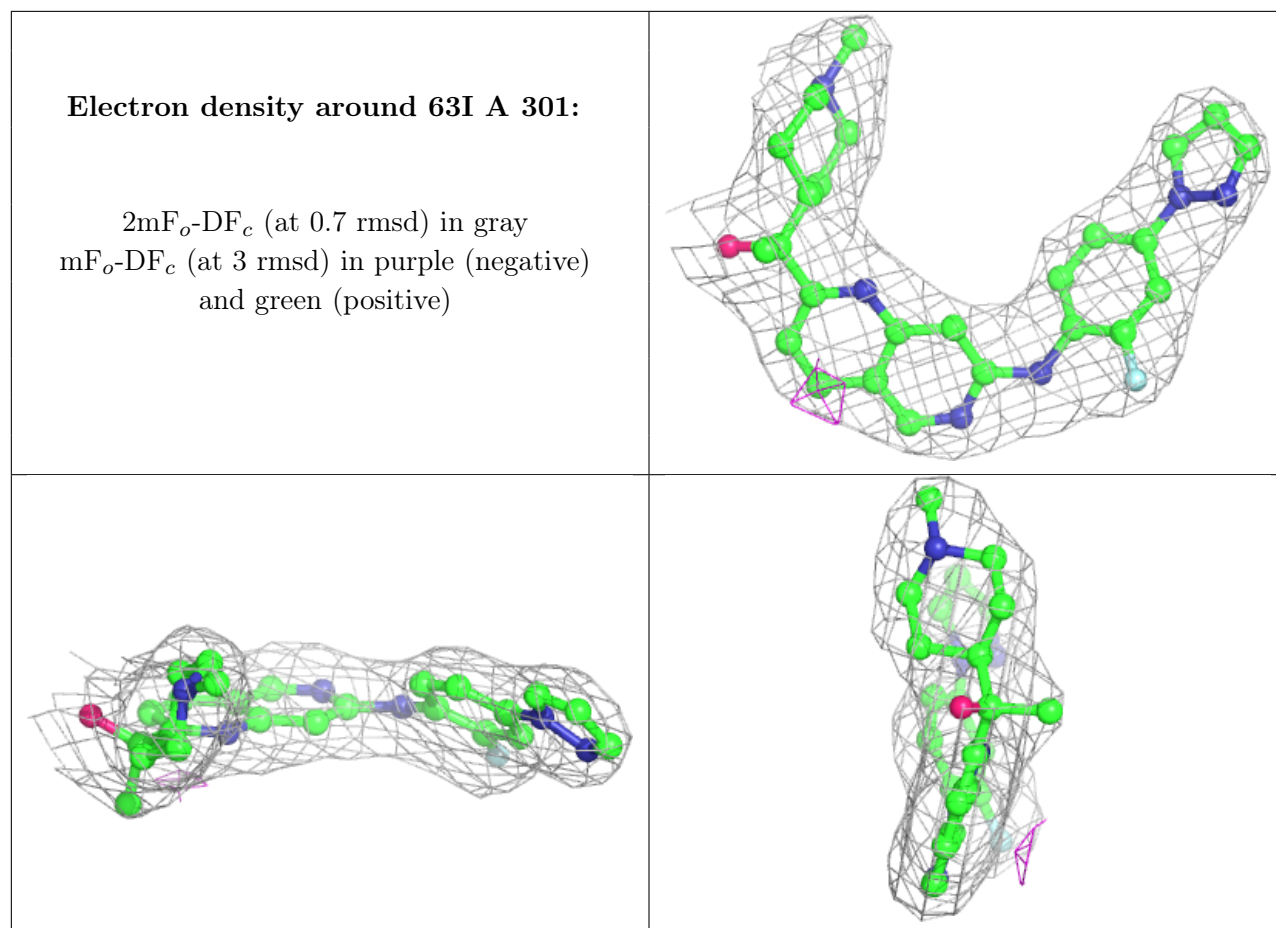
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 63I B 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)







## 6.5 Other polymers ⓘ

There are no such residues in this entry.