



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:26 am BST

PDB ID : 3K99  
Title : HSP90 N-terminal domain in complex with 4-(1,3-dihydro-2H-isoindol-2-ylcarbonyl)benzene-1,3-diol  
Authors : Gajiwala, K.S.; Davies II, J.F.  
Deposited on : 2009-10-15  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

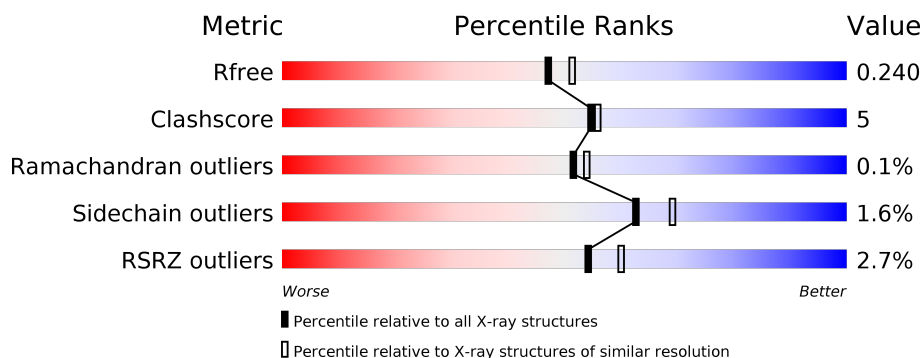
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	232	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	232	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	232	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div> </div>
1	D	232	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </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
2	PFT	A	901	-	X	-	-
2	PFT	B	901	-	X	-	-
2	PFT	C	901	-	X	-	-
2	PFT	D	901	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7303 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1720	1089	281	344	6			
1	B	216	Total	C	N	O	S	0	0	0
			1703	1080	278	339	6			
1	C	216	Total	C	N	O	S	0	0	0
			1703	1080	278	339	6			
1	D	217	Total	C	N	O	S	0	0	0
			1712	1085	280	341	6			

There are 60 discrepancies between the modelled and reference sequences:

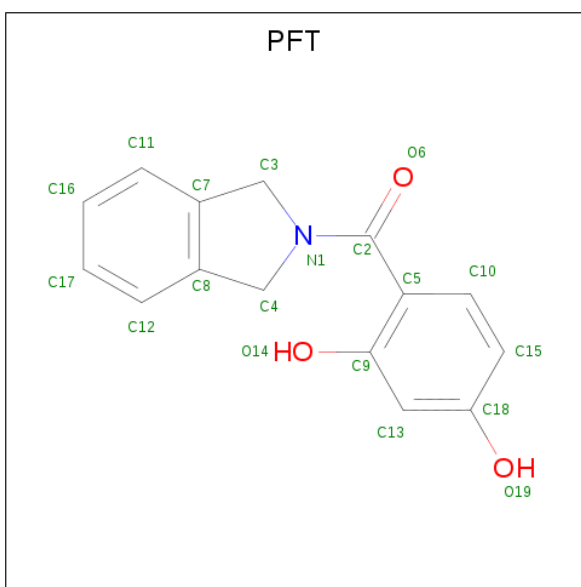
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	INITIATING METHIONINE	UNP P07900
A	226	LEU	-	EXPRESSION TAG	UNP P07900
A	227	GLU	-	EXPRESSION TAG	UNP P07900
A	228	HIS	-	EXPRESSION TAG	UNP P07900
A	229	HIS	-	EXPRESSION TAG	UNP P07900
A	230	HIS	-	EXPRESSION TAG	UNP P07900
A	231	HIS	-	EXPRESSION TAG	UNP P07900
A	232	HIS	-	EXPRESSION TAG	UNP P07900
A	233	HIS	-	EXPRESSION TAG	UNP P07900
A	234	HIS	-	EXPRESSION TAG	UNP P07900
A	235	HIS	-	EXPRESSION TAG	UNP P07900
A	236	HIS	-	EXPRESSION TAG	UNP P07900
A	237	HIS	-	EXPRESSION TAG	UNP P07900
A	238	HIS	-	EXPRESSION TAG	UNP P07900
A	239	HIS	-	EXPRESSION TAG	UNP P07900
B	8	MET	-	INITIATING METHIONINE	UNP P07900
B	226	LEU	-	EXPRESSION TAG	UNP P07900
B	227	GLU	-	EXPRESSION TAG	UNP P07900
B	228	HIS	-	EXPRESSION TAG	UNP P07900
B	229	HIS	-	EXPRESSION TAG	UNP P07900
B	230	HIS	-	EXPRESSION TAG	UNP P07900

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	HIS	-	EXPRESSION TAG	UNP P07900
B	232	HIS	-	EXPRESSION TAG	UNP P07900
B	233	HIS	-	EXPRESSION TAG	UNP P07900
B	234	HIS	-	EXPRESSION TAG	UNP P07900
B	235	HIS	-	EXPRESSION TAG	UNP P07900
B	236	HIS	-	EXPRESSION TAG	UNP P07900
B	237	HIS	-	EXPRESSION TAG	UNP P07900
B	238	HIS	-	EXPRESSION TAG	UNP P07900
B	239	HIS	-	EXPRESSION TAG	UNP P07900
C	8	MET	-	INITIATING METHIONINE	UNP P07900
C	226	LEU	-	EXPRESSION TAG	UNP P07900
C	227	GLU	-	EXPRESSION TAG	UNP P07900
C	228	HIS	-	EXPRESSION TAG	UNP P07900
C	229	HIS	-	EXPRESSION TAG	UNP P07900
C	230	HIS	-	EXPRESSION TAG	UNP P07900
C	231	HIS	-	EXPRESSION TAG	UNP P07900
C	232	HIS	-	EXPRESSION TAG	UNP P07900
C	233	HIS	-	EXPRESSION TAG	UNP P07900
C	234	HIS	-	EXPRESSION TAG	UNP P07900
C	235	HIS	-	EXPRESSION TAG	UNP P07900
C	236	HIS	-	EXPRESSION TAG	UNP P07900
C	237	HIS	-	EXPRESSION TAG	UNP P07900
C	238	HIS	-	EXPRESSION TAG	UNP P07900
C	239	HIS	-	EXPRESSION TAG	UNP P07900
D	8	MET	-	INITIATING METHIONINE	UNP P07900
D	226	LEU	-	EXPRESSION TAG	UNP P07900
D	227	GLU	-	EXPRESSION TAG	UNP P07900
D	228	HIS	-	EXPRESSION TAG	UNP P07900
D	229	HIS	-	EXPRESSION TAG	UNP P07900
D	230	HIS	-	EXPRESSION TAG	UNP P07900
D	231	HIS	-	EXPRESSION TAG	UNP P07900
D	232	HIS	-	EXPRESSION TAG	UNP P07900
D	233	HIS	-	EXPRESSION TAG	UNP P07900
D	234	HIS	-	EXPRESSION TAG	UNP P07900
D	235	HIS	-	EXPRESSION TAG	UNP P07900
D	236	HIS	-	EXPRESSION TAG	UNP P07900
D	237	HIS	-	EXPRESSION TAG	UNP P07900
D	238	HIS	-	EXPRESSION TAG	UNP P07900
D	239	HIS	-	EXPRESSION TAG	UNP P07900

- Molecule 2 is 4-(1,3-dihydro-2H-isoindol-2-ylcarbonyl)benzene-1,3-diol (three-letter code: PFT) (formula: C<sub>15</sub>H<sub>13</sub>NO<sub>3</sub>).



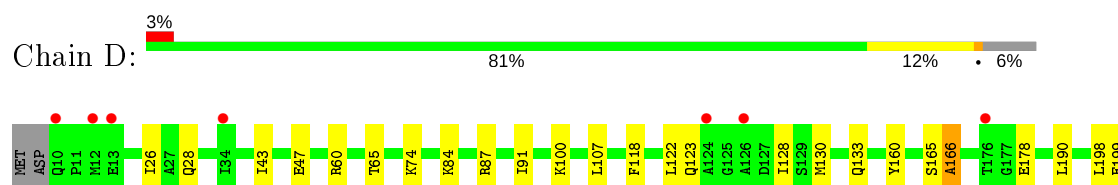
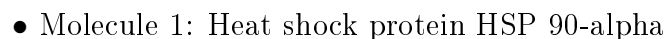
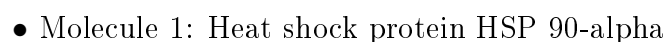
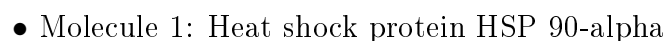
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	15	1	3		
2	B	1	Total	C	N	O	0	0
			19	15	1	3		
2	C	1	Total	C	N	O	0	0
			19	15	1	3		
2	D	1	Total	C	N	O	0	0
			19	15	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	87	Total	O	0	0
			87	87		
3	C	90	Total	O	0	0
			90	90		
3	D	97	Total	O	0	0
			97	97		



- Molecule 1: Heat shock protein HSP 90-alpha







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.77Å 82.96Å 219.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.95-2.10) 95.6 (19.95-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.09Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.204 , 0.245 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	2540 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0263e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PFT

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	0.29	0/1747	0.46	0/2355
1	B	0.29	0/1730	0.48	0/2331
1	C	0.28	0/1730	0.49	0/2331
1	D	0.29	0/1739	0.47	0/2344
All	All	0.29	0/6946	0.48	0/9361

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	1720	0	1710	22	0
1	B	1703	0	1699	11	0
1	C	1703	0	1699	23	0
1	D	1712	0	1706	22	0
2	A	19	0	12	0	0
2	B	19	0	12	0	0
2	C	19	0	12	0	0
2	D	19	0	12	0	0
3	A	115	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	87	0	0	2	0
3	C	90	0	0	3	0
3	D	97	0	0	0	0
All	All	7303	0	6862	72	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 5.

All (72) 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:C:212:GLN:CD	1:C:212:GLN:H	2.03	0.62
1:C:176:THR:O	1:C:176:THR:HG22	2.00	0.62
1:C:84:LYS:HA	1:C:198:LEU:HD13	1.84	0.60
1:B:14:GLU:HG3	1:B:14:GLU:O	2.02	0.59
1:D:60:ARG:HG2	1:D:60:ARG:HH11	1.67	0.59
1:A:23:GLN:NE2	1:A:25:GLU:HB2	2.18	0.58
1:A:109:THR:HG21	3:A:317:HOH:O	2.05	0.56
1:D:28:GLN:HE21	1:D:123:GLN:NE2	2.03	0.56
1:A:62:GLU:OE1	1:A:69:LYS:HE2	2.07	0.54
1:A:202:ARG:O	1:A:205:GLU:HG2	2.08	0.54
1:A:200:GLU:O	1:A:204:LYS:HG3	2.08	0.54
1:B:204:LYS:HG2	1:D:226:LEU:HD22	1.91	0.53
1:D:107:LEU:N	1:D:107:LEU:HD12	2.25	0.52
1:C:103:LEU:O	1:C:107:LEU:HB2	2.10	0.52
1:D:28:GLN:NE2	1:D:123:GLN:NE2	2.57	0.52
1:A:165:SER:O	1:A:166:ALA:HB3	2.10	0.51
1:C:127:ASP:OD1	1:C:129:SER:HB2	2.11	0.51
1:A:58:LYS:NZ	1:A:62:GLU:OE2	2.44	0.51
1:C:32:LEU:HD21	1:C:123:GLN:HG3	1.93	0.50
1:D:91:ILE:HD12	1:D:91:ILE:N	2.28	0.48
1:A:116:LYS:NZ	1:A:116:LYS:HB2	2.28	0.48
1:A:9:ASP:HB2	3:C:301:HOH:O	2.13	0.48
1:C:92:VAL:HG22	1:C:185:LYS:HG3	1.95	0.48
1:A:19:THR:O	1:C:12:MET:HB2	2.13	0.48
1:D:205:GLU:HG3	1:D:206:ILE:N	2.28	0.48
1:B:112:LYS:HB3	3:B:305:HOH:O	2.13	0.48
1:B:91:ILE:N	1:B:91:ILE:HD12	2.29	0.48
1:D:128:ILE:O	1:D:128:ILE:HG13	2.13	0.47
1:D:60:ARG:HG2	1:D:60:ARG:NH1	2.30	0.47
1:D:165:SER:O	1:D:166:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HD3	1:A:210:HIS:HB3	1.97	0.46
1:A:56:LEU:HD22	1:A:76:LEU:HB3	1.98	0.45
1:D:26:ILE:HD12	1:D:26:ILE:N	2.31	0.45
1:D:200:GLU:HG2	1:D:204:LYS:HD3	1.98	0.45
1:A:20:PHE:HB2	1:A:170:PHE:CZ	2.52	0.45
1:C:155:ASN:O	1:C:156:ASP:HB2	2.16	0.45
1:C:128:ILE:HG12	1:C:143:LEU:HD11	1.98	0.45
1:B:165:SER:O	1:B:166:ALA:HB3	2.17	0.45
1:A:48:LEU:HD13	1:A:91:ILE:HD13	2.00	0.44
1:C:91:ILE:HD12	1:C:91:ILE:N	2.33	0.44
1:C:103:LEU:HD22	1:C:162:TRP:HB2	2.00	0.43
1:D:130:MET:HE2	1:D:133:GLN:HG3	2.00	0.43
1:A:77:HIS:HE1	3:A:250:HOH:O	1.99	0.43
1:A:21:ALA:HB2	1:C:12:MET:CE	2.49	0.43
1:C:213:PHE:HB2	3:C:371:HOH:O	2.17	0.43
1:D:84:LYS:NZ	1:D:199:GLU:OE2	2.44	0.43
1:D:100:LYS:HB2	1:D:160:TYR:CZ	2.54	0.42
1:B:92:VAL:HG22	1:B:185:LYS:HD3	2.00	0.42
1:C:87:ARG:NH1	1:C:192:GLU:HG2	2.34	0.42
1:B:84:LYS:HA	1:B:198:LEU:HD13	2.00	0.42
1:D:190:LEU:HD12	1:D:198:LEU:HG	2.01	0.42
1:B:36:THR:HB	1:B:38:TYR:CE1	2.53	0.42
1:C:58:LYS:O	1:C:62:GLU:HG3	2.20	0.42
1:C:48:LEU:HD13	1:C:91:ILE:HD13	2.01	0.42
1:A:84:LYS:HA	1:A:198:LEU:HD13	2.02	0.41
1:C:159:GLN:HG2	1:C:175:ASP:HB3	2.02	0.41
1:D:43:ILE:O	1:D:47:GLU:HG2	2.20	0.41
1:D:118:PHE:CE2	1:D:122:LEU:HD11	2.56	0.41
1:A:12:MET:SD	1:C:21:ALA:HB2	2.60	0.41
1:A:43:ILE:O	1:A:47:GLU:HG2	2.20	0.41
1:D:74:LYS:HE3	1:D:74:LYS:HB3	1.84	0.41
1:A:18:GLU:HG2	1:C:14:GLU:OE2	2.21	0.41
1:C:189:HIS:HE1	3:C:326:HOH:O	2.03	0.41
1:D:130:MET:CE	1:D:133:GLN:HG3	2.51	0.41
1:B:144:VAL:HA	1:B:194:GLN:HG3	2.03	0.41
1:B:77:HIS:HE1	3:B:307:HOH:O	2.03	0.41
1:A:16:GLU:HB3	1:C:14:GLU:OE1	2.21	0.41
1:B:196:GLU:O	1:B:199:GLU:HB2	2.21	0.40
1:A:212:GLN:HB2	3:A:262:HOH:O	2.20	0.40
1:D:65:THR:HG22	1:D:65:THR:O	2.22	0.40
1:C:205:GLU:O	1:C:209:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HD2	1:D:190:LEU:O	2.22	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	216/232 (93%)	213 (99%)	3 (1%)	0	100	100
1	B	214/232 (92%)	208 (97%)	6 (3%)	0	100	100
1	C	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
1	D	215/232 (93%)	207 (96%)	7 (3%)	1 (0%)	29	26
All	All	859/928 (93%)	837 (97%)	21 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	166	ALA

### 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	189/203 (93%)	186 (98%)	3 (2%)	62	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	187/203 (92%)	182 (97%)	5 (3%)	44	48
1	C	187/203 (92%)	185 (99%)	2 (1%)	73	79
1	D	188/203 (93%)	186 (99%)	2 (1%)	73	79
All	All	751/812 (92%)	739 (98%)	12 (2%)	62	69

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	74	LYS
1	A	77	HIS
1	B	14	GLU
1	B	123	GLN
1	B	201	ARG
1	B	224	LYS
1	B	225	GLU
1	C	212	GLN
1	C	224	LYS
1	D	178	GLU
1	D	205	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	189	HIS
1	C	133	GLN
1	C	189	HIS
1	D	28	GLN
1	D	85	GLN
1	D	212	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	PFT	C	901	-	21,21,21	3.42	15 (71%)	27,30,30	4.42	17 (62%)
2	PFT	D	901	-	21,21,21	3.45	15 (71%)	27,30,30	4.54	17 (62%)
2	PFT	A	901	-	21,21,21	3.44	15 (71%)	27,30,30	4.60	17 (62%)
2	PFT	B	901	-	21,21,21	3.38	15 (71%)	27,30,30	4.42	17 (62%)

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	PFT	C	901	-	-	0/8/16/16	0/3/3/3
2	PFT	D	901	-	-	0/8/16/16	0/3/3/3
2	PFT	A	901	-	-	0/8/16/16	0/3/3/3
2	PFT	B	901	-	-	0/8/16/16	0/3/3/3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	PFT	C4-N1	6.27	1.56	1.46
2	B	901	PFT	C4-N1	6.24	1.56	1.46
2	A	901	PFT	C4-N1	6.11	1.56	1.46
2	D	901	PFT	C4-N1	5.96	1.55	1.46
2	A	901	PFT	C3-C7	5.67	1.57	1.50
2	D	901	PFT	C3-C7	5.34	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	PFT	C3-C7	5.14	1.57	1.50
2	C	901	PFT	C3-C7	5.12	1.57	1.50
2	C	901	PFT	C13-C18	4.85	1.46	1.39
2	A	901	PFT	C15-C18	4.78	1.48	1.38
2	B	901	PFT	C16-C11	4.71	1.48	1.38
2	B	901	PFT	C13-C18	4.62	1.46	1.39
2	D	901	PFT	C16-C11	4.61	1.48	1.38
2	D	901	PFT	C13-C18	4.60	1.46	1.39
2	C	901	PFT	C16-C11	4.60	1.48	1.38
2	D	901	PFT	C3-N1	4.55	1.53	1.46
2	A	901	PFT	C16-C11	4.55	1.48	1.38
2	D	901	PFT	C2-N1	4.50	1.44	1.34
2	B	901	PFT	C2-N1	4.48	1.44	1.34
2	C	901	PFT	C2-N1	4.47	1.44	1.34
2	C	901	PFT	C15-C18	4.46	1.47	1.38
2	D	901	PFT	C15-C18	4.45	1.47	1.38
2	A	901	PFT	C3-N1	4.38	1.53	1.46
2	A	901	PFT	C2-N1	4.33	1.44	1.34
2	B	901	PFT	C15-C18	4.25	1.47	1.38
2	B	901	PFT	C3-N1	4.25	1.53	1.46
2	A	901	PFT	C13-C18	4.10	1.45	1.39
2	C	901	PFT	C3-N1	3.87	1.52	1.46
2	A	901	PFT	C8-C7	3.81	1.46	1.39
2	D	901	PFT	C8-C7	3.73	1.46	1.39
2	C	901	PFT	C8-C7	3.64	1.46	1.39
2	B	901	PFT	C8-C7	3.63	1.46	1.39
2	D	901	PFT	C17-C16	3.61	1.47	1.38
2	A	901	PFT	C17-C16	3.61	1.47	1.38
2	B	901	PFT	C17-C16	3.59	1.47	1.38
2	D	901	PFT	C5-C9	3.59	1.46	1.40
2	C	901	PFT	C17-C16	3.55	1.47	1.38
2	A	901	PFT	C5-C9	3.47	1.46	1.40
2	A	901	PFT	C12-C8	3.06	1.44	1.39
2	C	901	PFT	C11-C7	3.02	1.44	1.39
2	B	901	PFT	C12-C8	3.00	1.44	1.39
2	D	901	PFT	C11-C7	2.94	1.44	1.39
2	C	901	PFT	C12-C8	2.92	1.44	1.39
2	B	901	PFT	C11-C7	2.91	1.44	1.39
2	D	901	PFT	C12-C8	2.90	1.44	1.39
2	C	901	PFT	C5-C9	2.83	1.45	1.40
2	B	901	PFT	C5-C9	2.79	1.45	1.40
2	C	901	PFT	C13-C9	2.77	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	PFT	C11-C7	2.65	1.44	1.39
2	C	901	PFT	C10-C5	2.65	1.44	1.39
2	B	901	PFT	C13-C9	2.44	1.42	1.38
2	D	901	PFT	C13-C9	2.40	1.42	1.38
2	A	901	PFT	C4-C8	-2.38	1.47	1.50
2	B	901	PFT	C10-C5	2.34	1.43	1.39
2	D	901	PFT	C10-C5	2.31	1.43	1.39
2	C	901	PFT	C5-C2	2.29	1.54	1.50
2	D	901	PFT	C4-C8	-2.26	1.47	1.50
2	A	901	PFT	C13-C9	2.17	1.42	1.38
2	B	901	PFT	O19-C18	-2.07	1.32	1.37
2	A	901	PFT	O19-C18	-2.07	1.32	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	PFT	C9-C13-C18	-13.66	107.33	119.70
2	A	901	PFT	C9-C13-C18	-13.54	107.45	119.70
2	C	901	PFT	C9-C13-C18	-13.38	107.59	119.70
2	B	901	PFT	C9-C13-C18	-13.35	107.62	119.70
2	A	901	PFT	C8-C4-N1	8.80	106.62	102.46
2	D	901	PFT	C8-C4-N1	8.58	106.52	102.46
2	D	901	PFT	C15-C18-C13	8.20	129.16	120.17
2	A	901	PFT	C15-C18-C13	8.19	129.15	120.17
2	B	901	PFT	C15-C18-C13	8.14	129.09	120.17
2	C	901	PFT	C15-C18-C13	8.07	129.02	120.17
2	B	901	PFT	C8-C4-N1	7.71	106.11	102.46
2	C	901	PFT	C8-C4-N1	7.49	106.00	102.46
2	A	901	PFT	O6-C2-C5	5.77	131.68	120.06
2	D	901	PFT	O6-C2-C5	5.68	131.51	120.06
2	B	901	PFT	O6-C2-C5	5.65	131.44	120.06
2	C	901	PFT	O6-C2-C5	5.58	131.30	120.06
2	C	901	PFT	O6-C2-N1	-5.48	113.27	122.34
2	B	901	PFT	O6-C2-N1	-5.33	113.53	122.34
2	A	901	PFT	C12-C8-C7	5.33	126.36	120.11
2	D	901	PFT	O6-C2-N1	-5.24	113.68	122.34
2	A	901	PFT	O6-C2-N1	-5.23	113.69	122.34
2	A	901	PFT	C13-C9-C5	5.12	125.87	120.60
2	D	901	PFT	C12-C8-C7	5.12	126.11	120.11
2	B	901	PFT	C12-C8-C7	5.08	126.07	120.11
2	C	901	PFT	C13-C9-C5	5.02	125.76	120.60
2	D	901	PFT	C13-C9-C5	5.01	125.76	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	PFT	C12-C8-C7	4.97	125.94	120.11
2	B	901	PFT	C13-C9-C5	4.95	125.69	120.60
2	A	901	PFT	C10-C5-C9	4.66	123.99	118.15
2	B	901	PFT	C10-C5-C9	4.48	123.76	118.15
2	C	901	PFT	C10-C5-C9	4.47	123.75	118.15
2	D	901	PFT	C10-C5-C9	4.44	123.71	118.15
2	A	901	PFT	C15-C10-C5	-4.31	113.94	120.94
2	D	901	PFT	C15-C10-C5	-4.15	114.20	120.94
2	A	901	PFT	C9-C5-C2	-4.03	111.16	119.89
2	C	901	PFT	C15-C10-C5	-4.01	114.44	120.94
2	B	901	PFT	C15-C10-C5	-3.98	114.49	120.94
2	A	901	PFT	C11-C7-C8	-3.93	115.51	120.11
2	C	901	PFT	C9-C5-C2	-3.85	111.54	119.89
2	B	901	PFT	C11-C7-C8	-3.71	115.76	120.11
2	D	901	PFT	C11-C7-C8	-3.64	115.85	120.11
2	D	901	PFT	C9-C5-C2	-3.63	112.03	119.89
2	C	901	PFT	C11-C7-C8	-3.53	115.98	120.11
2	B	901	PFT	C9-C5-C2	-3.47	112.37	119.89
2	D	901	PFT	O14-C9-C13	-3.43	110.27	119.46
2	A	901	PFT	O14-C9-C13	-3.43	110.28	119.46
2	B	901	PFT	O14-C9-C13	-3.33	110.54	119.46
2	C	901	PFT	O14-C9-C13	-3.23	110.82	119.46
2	A	901	PFT	C4-C8-C12	-2.93	123.07	128.85
2	D	901	PFT	C4-C8-C12	-2.90	123.13	128.85
2	B	901	PFT	C4-C8-C12	-2.82	123.28	128.85
2	A	901	PFT	C10-C5-C2	2.81	124.85	119.26
2	C	901	PFT	C4-C8-C12	-2.75	123.42	128.85
2	A	901	PFT	C3-C7-C11	2.75	134.26	128.85
2	C	901	PFT	C10-C5-C2	2.73	124.70	119.26
2	D	901	PFT	C3-C7-C11	2.65	134.07	128.85
2	B	901	PFT	C3-C7-C11	2.62	134.02	128.85
2	C	901	PFT	C3-C7-C11	2.57	133.92	128.85
2	D	901	PFT	C10-C5-C2	2.51	124.26	119.26
2	A	901	PFT	C17-C12-C8	-2.48	117.19	120.89
2	D	901	PFT	C17-C12-C8	-2.46	117.22	120.89
2	C	901	PFT	C17-C12-C8	-2.40	117.31	120.89
2	B	901	PFT	C17-C12-C8	-2.32	117.43	120.89
2	B	901	PFT	C10-C5-C2	2.32	123.87	119.26
2	A	901	PFT	C5-C2-N1	-2.30	114.61	118.28
2	C	901	PFT	C7-C3-N1	2.26	103.53	102.46
2	D	901	PFT	C5-C2-N1	-2.18	114.80	118.28
2	B	901	PFT	C5-C2-N1	-2.04	115.03	118.28

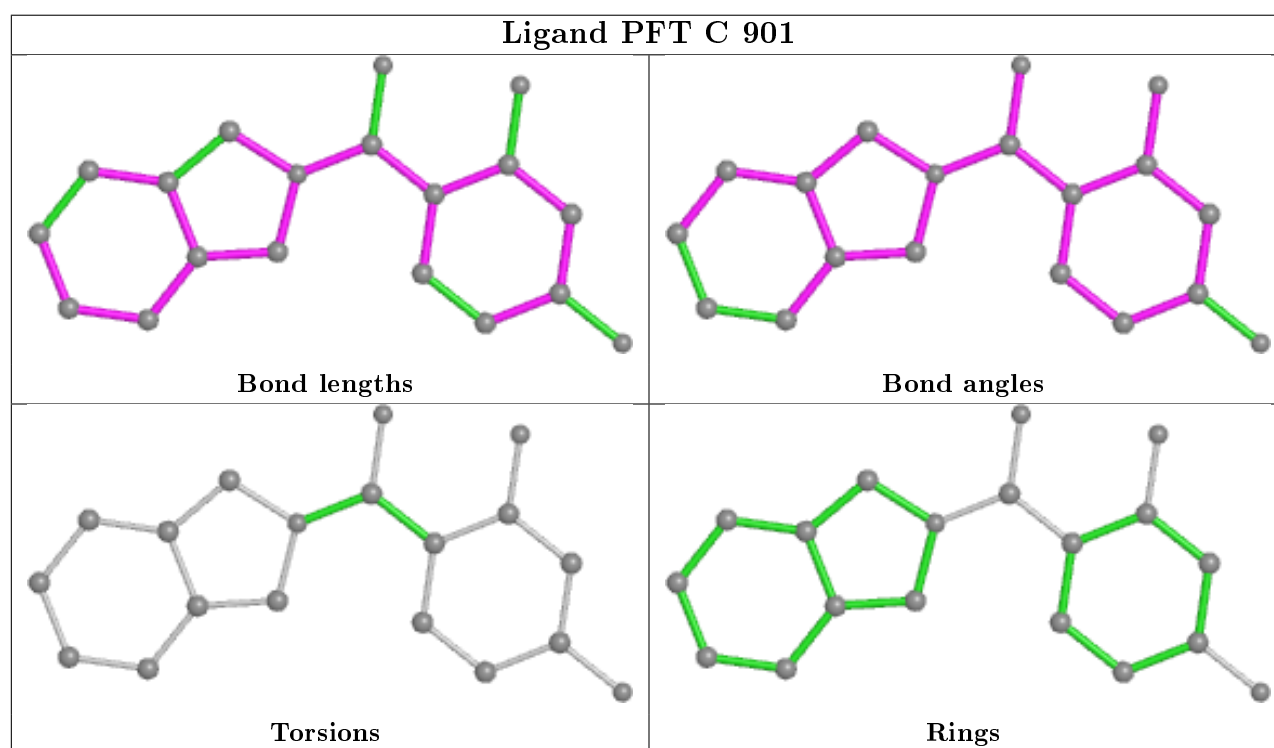
There are no chirality outliers.

There are no torsion outliers.

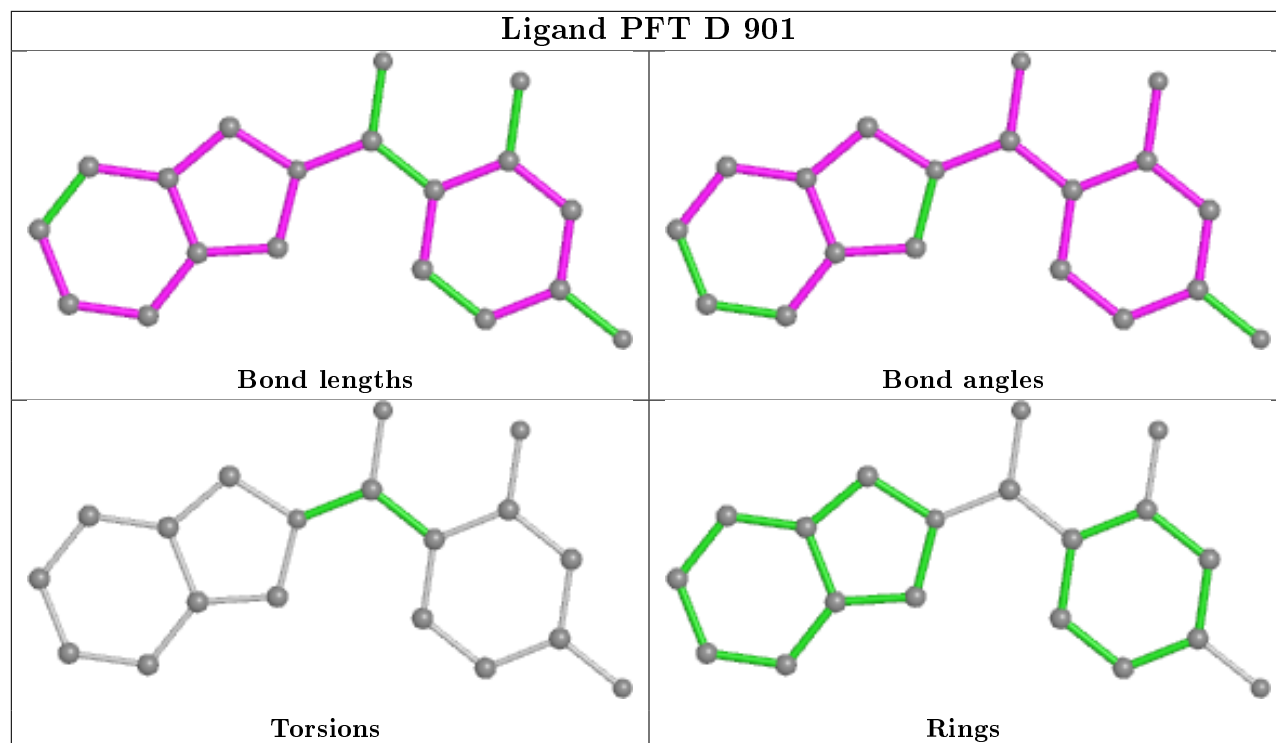
There are no ring outliers.

No monomer is involved in short contacts.

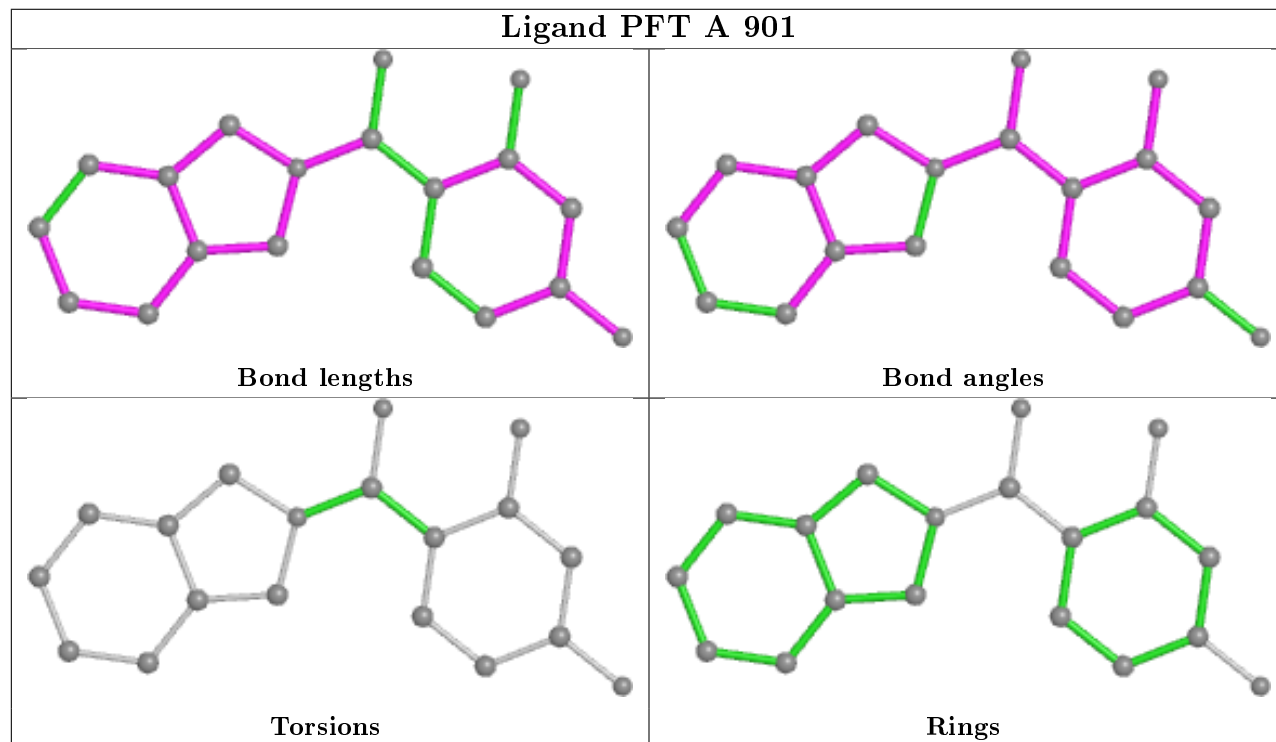
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

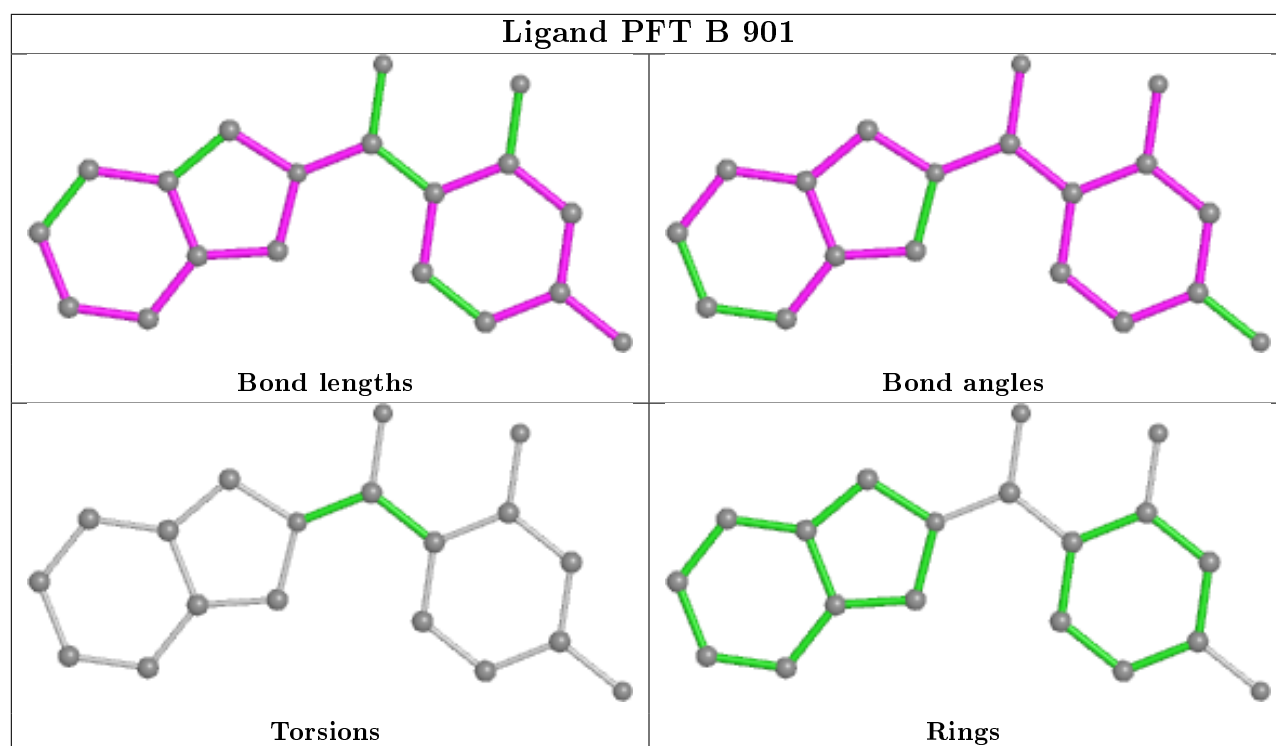


## Ligand PFT D 901



## Ligand PFT A 901





## 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	218/232 (93%)	-0.07	4 (1%) 68 72	15, 26, 41, 52	0
1	B	216/232 (93%)	-0.00	3 (1%) 75 78	16, 28, 46, 53	0
1	C	216/232 (93%)	0.06	8 (3%) 41 48	16, 29, 50, 59	0
1	D	217/232 (93%)	0.01	8 (3%) 41 48	16, 29, 43, 55	0
All	All	867/928 (93%)	-0.00	23 (2%) 54 60	15, 28, 45, 59	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	PHE	5.3
1	A	124	ALA	4.2
1	C	213	PHE	4.1
1	D	10	GLN	3.8
1	D	12	MET	3.3
1	D	126	ALA	3.2
1	C	39	SER	3.1
1	C	12	MET	3.1
1	A	166	ALA	2.9
1	D	124	ALA	2.8
1	A	65	THR	2.5
1	D	176	THR	2.5
1	B	39	SER	2.5
1	C	14	GLU	2.5
1	D	13	GLU	2.2
1	A	212	GLN	2.1
1	C	123	GLN	2.1
1	C	124	ALA	2.1
1	C	176	THR	2.1
1	D	212	GLN	2.0
1	B	201	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	181	GLY	2.0
1	D	34	ILE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

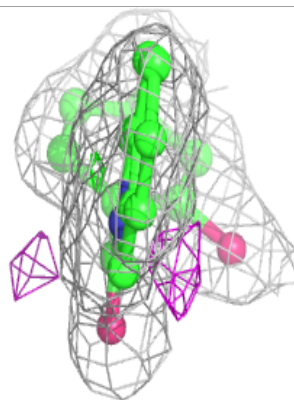
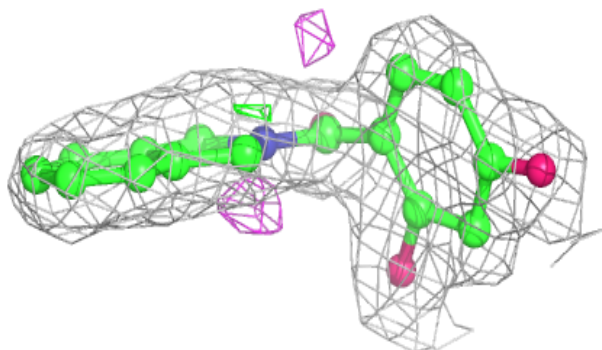
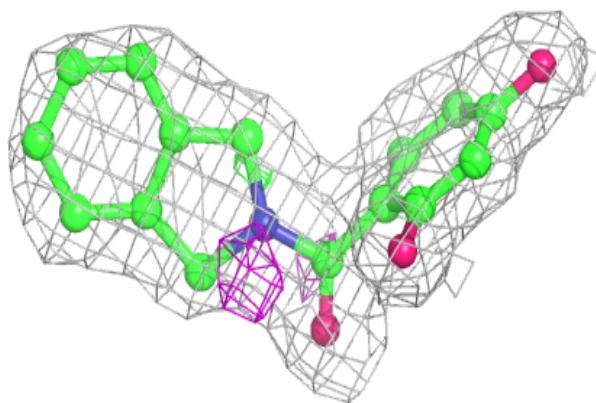
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	PFT	D	901	19/19	0.90	0.13	19,21,23,25	0
2	PFT	A	901	19/19	0.93	0.12	14,18,20,21	0
2	PFT	B	901	19/19	0.93	0.12	17,19,22,24	0
2	PFT	C	901	19/19	0.95	0.10	16,18,21,21	0

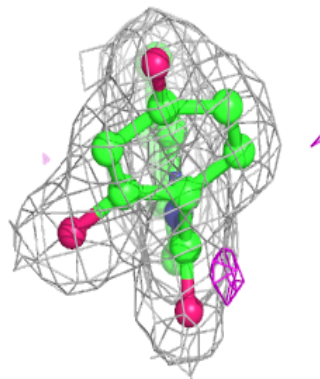
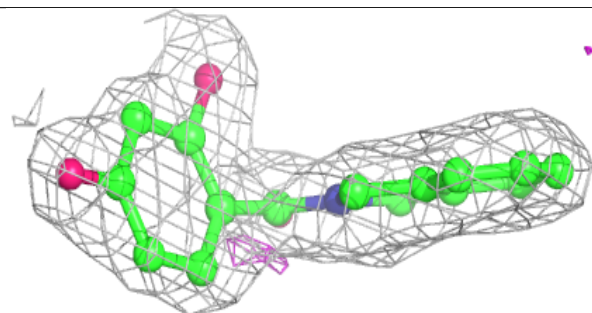
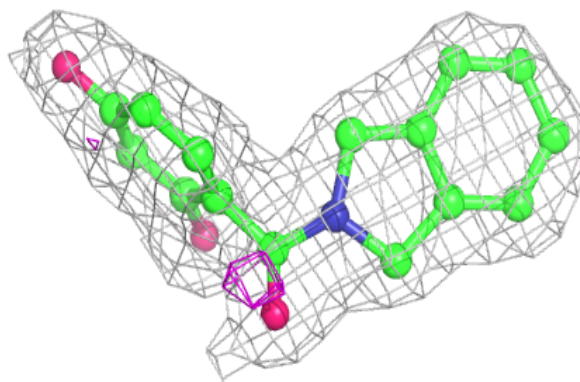
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PFT D 901:**

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

**Electron density around PFT A 901:**

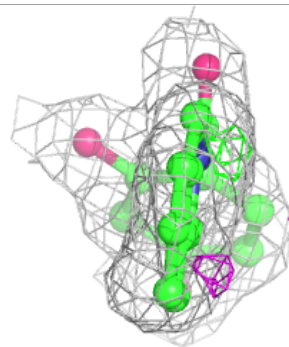
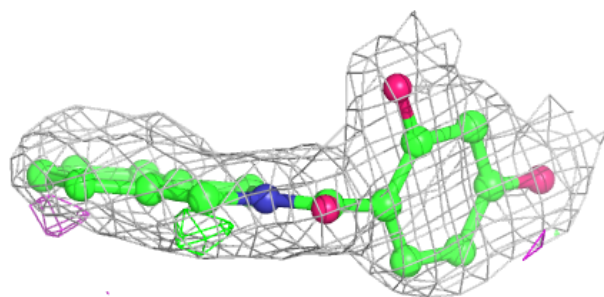
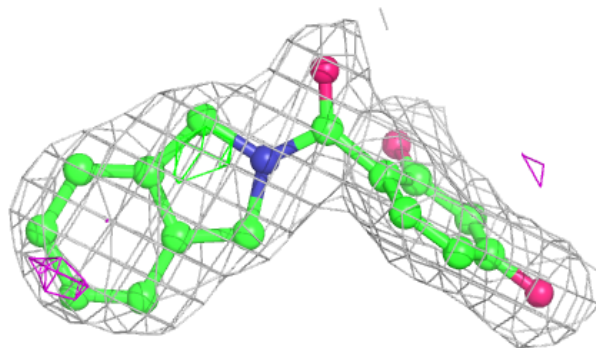
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



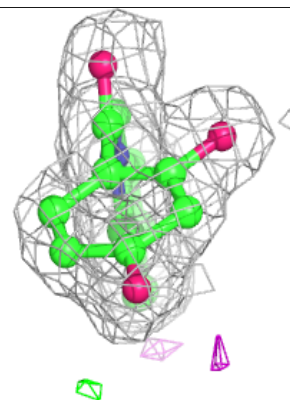
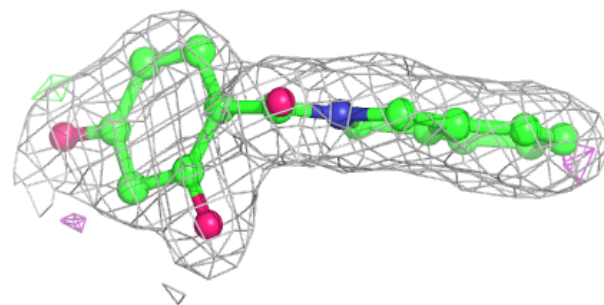
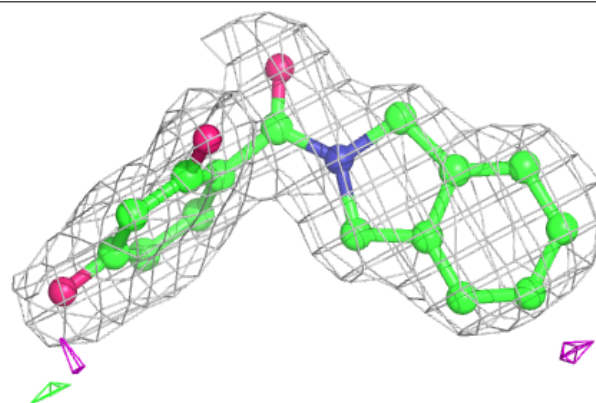


**Electron density around PFT B 901:**

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

**Electron density around PFT C 901:**

$2mF_o-DF_c$  (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.