



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:09 AM UTC

PDB ID : 6FUG / pdb_00006fug
Title : Complement factor D in complex with the inhibitor 3-((3-((3-(aminomethyl)phenyl)amino)-1H-pyrazolo[3,4-d]pyrimidin-4-yl)amino)phenol
Authors : Mac Sweeney, A.; Ostermann, N.; Vulpetti, A.; Maibaum, J.; Erbel, P.; Lorthiois, E.; Yoon, T.; Randl, S.; Ruedisser, S.
Deposited on : 2018-02-27
Resolution : 2.21 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

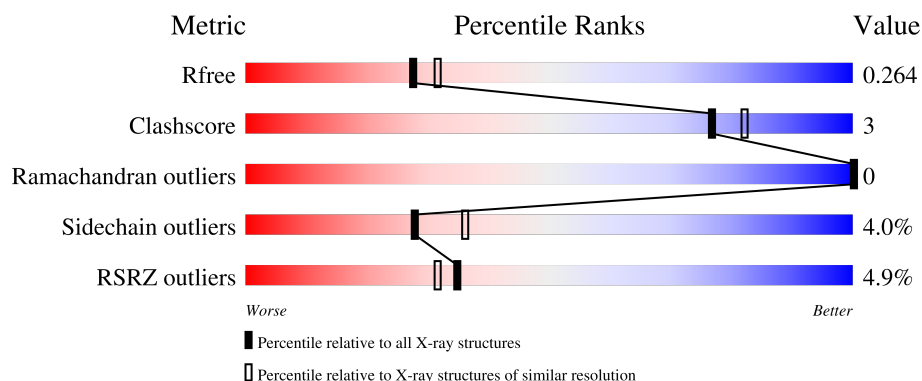
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	2% 85% 7% • 7%
1	B	232	4% 85% 6% 9%
1	C	232	6% 87% 6% • 6%
1	D	232	4% 86% 6% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	232	8% 83% 8% 8%
1	F	232	4% 87% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10121 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 Complement factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	2	0
			1615	1005	301	299	10			
1	B	211	Total	C	N	O	S	0	6	0
			1613	1008	295	299	11			
1	C	218	Total	C	N	O	S	0	2	0
			1617	1007	297	303	10			
1	D	214	Total	C	N	O	S	0	3	0
			1611	1005	297	298	11			
1	E	213	Total	C	N	O	S	0	4	0
			1616	1008	299	299	10			
1	F	213	Total	C	N	O	S	0	4	0
			1608	1004	296	298	10			

There are 24 discrepancies between the modelled and reference sequences:

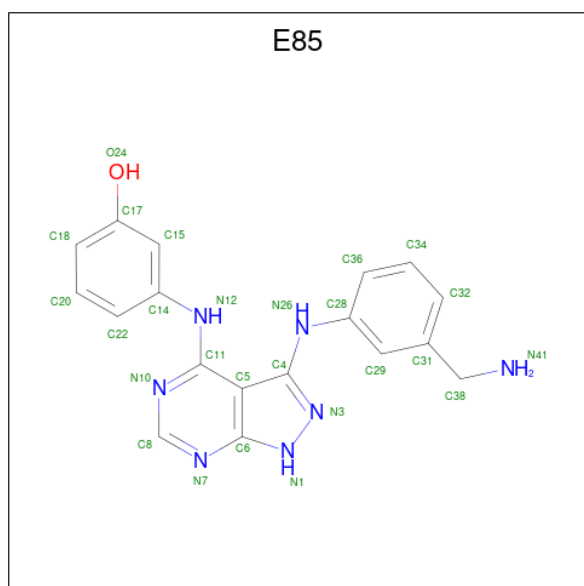
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	SER	-	expression tag	UNP P00746
A	245	ALA	-	expression tag	UNP P00746
A	246	ALA	-	expression tag	UNP P00746
A	247	ALA	-	expression tag	UNP P00746
B	244	SER	-	expression tag	UNP P00746
B	245	ALA	-	expression tag	UNP P00746
B	246	ALA	-	expression tag	UNP P00746
B	247	ALA	-	expression tag	UNP P00746
C	244	SER	-	expression tag	UNP P00746
C	245	ALA	-	expression tag	UNP P00746
C	246	ALA	-	expression tag	UNP P00746
C	247	ALA	-	expression tag	UNP P00746
D	244	SER	-	expression tag	UNP P00746
D	245	ALA	-	expression tag	UNP P00746
D	246	ALA	-	expression tag	UNP P00746
D	247	ALA	-	expression tag	UNP P00746
E	244	SER	-	expression tag	UNP P00746

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	245	ALA	-	expression tag	UNP P00746
E	246	ALA	-	expression tag	UNP P00746
E	247	ALA	-	expression tag	UNP P00746
F	244	SER	-	expression tag	UNP P00746
F	245	ALA	-	expression tag	UNP P00746
F	246	ALA	-	expression tag	UNP P00746
F	247	ALA	-	expression tag	UNP P00746

- Molecule 2 is 3-[[3-[[3-(aminomethyl)phenyl]amino]-1 {H}-pyrazolo[3,4-d]pyrimidin-4-yl]amino]phenol (CCD ID: E85) (formula: C₁₈H₁₇N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	7	1		
2	B	1	Total	C	N	O	0	0
			26	18	7	1		
2	C	1	Total	C	N	O	0	0
			26	18	7	1		
2	D	1	Total	C	N	O	0	0
			26	18	7	1		
2	E	1	Total	C	N	O	0	0
			26	18	7	1		
2	F	1	Total	C	N	O	0	0
			26	18	7	1		

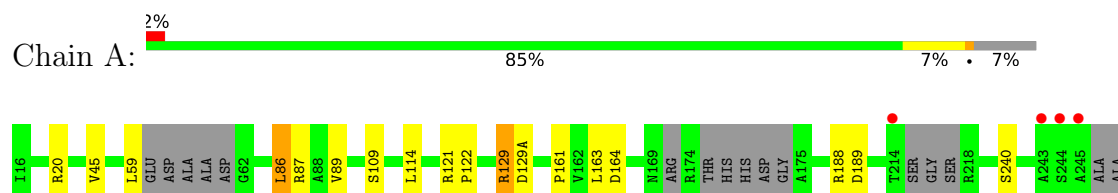
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	50	Total 50	O 50	0	0
3	C	49	Total 49	O 49	0	0
3	D	45	Total 45	O 45	0	0
3	E	39	Total 39	O 39	0	0
3	F	45	Total 45	O 45	0	0

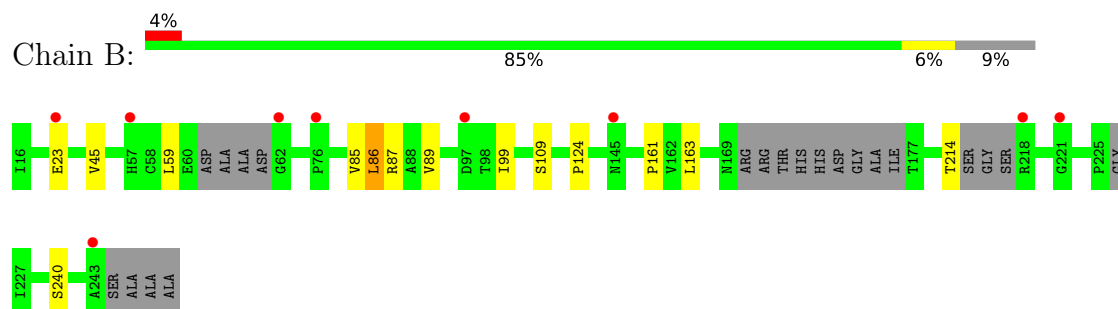
3 Residue-property plots

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.

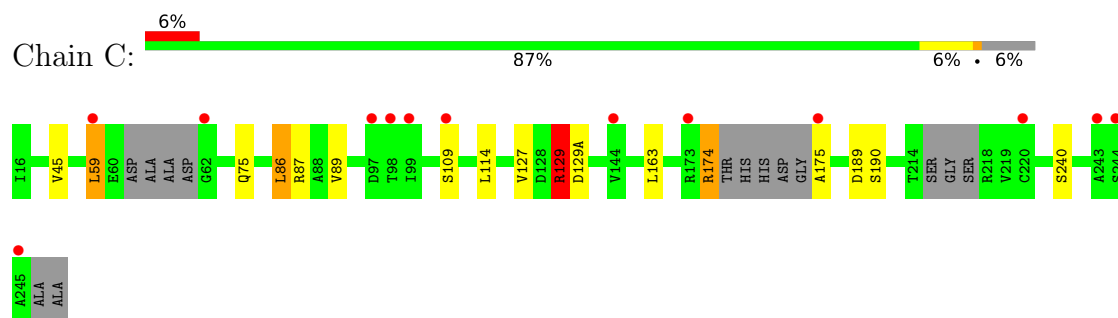
- Molecule 1: Complement factor D



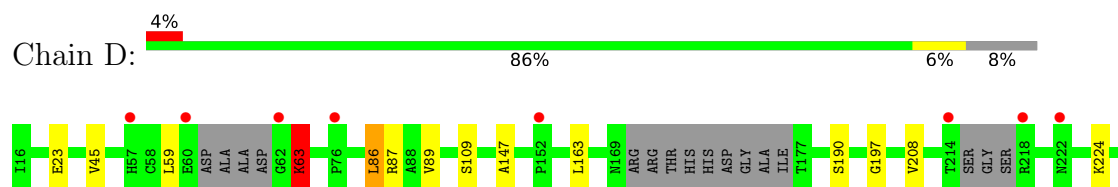
- Molecule 1: Complement factor D



- Molecule 1: Complement factor D

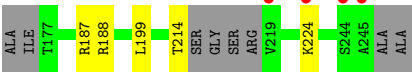
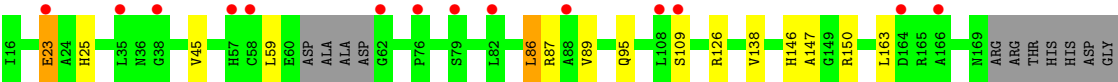
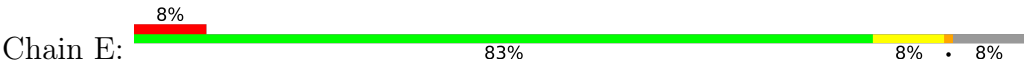


- Molecule 1: Complement factor D

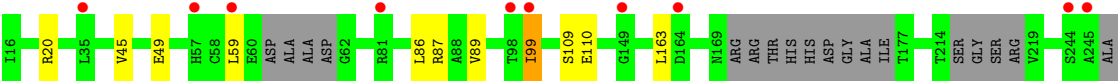
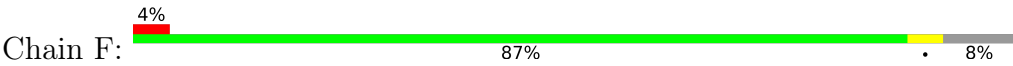




● Molecule 1: Complement factor D



● Molecule 1: Complement factor D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.52Å 68.48Å 73.38Å 95.21° 116.70° 102.43°	Depositor
Resolution (Å)	46.11 – 2.21 46.11 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.6 (46.11-2.21) 94.6 (46.11-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.221 , 0.259 0.225 , 0.264	Depositor DCC
R_{free} test set	2617 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10121	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.27 % 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 7.2723e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E85

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	0.86	0/1648	0.91	1/2242 (0.0%)
1	B	0.82	0/1651	0.86	0/2245
1	C	0.85	1/1650 (0.1%)	0.93	3/2247 (0.1%)
1	D	0.80	0/1644	0.89	1/2236 (0.0%)
1	E	0.85	1/1652 (0.1%)	0.91	1/2247 (0.0%)
1	F	0.82	0/1644	0.89	0/2237
All	All	0.83	2/9889 (0.0%)	0.90	6/13454 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	147	ALA	C-N	5.85	1.41	1.33
1	C	174	ARG	CA-C	5.00	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ARG	CA-CB-CG	-5.46	103.17	114.10
1	C	175	ALA	N-CA-C	5.42	119.61	112.89
1	E	23	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	20	ARG	CA-CB-CG	5.13	124.36	114.10
1	D	63	LYS	CA-CB-CG	5.04	124.17	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	LEU	N-CA-C	5.02	118.55	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	174	ARG	Peptide

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	1615	0	1602	11	0
1	B	1613	0	1605	8	0
1	C	1617	0	1588	13	0
1	D	1611	0	1600	13	0
1	E	1616	0	1616	12	0
1	F	1608	0	1600	6	0
2	A	26	0	0	2	0
2	B	26	0	0	0	0
2	C	26	0	0	3	0
2	D	26	0	0	2	0
2	E	26	0	0	1	0
2	F	26	0	0	2	0
3	A	57	0	0	2	0
3	B	50	0	0	2	0
3	C	49	0	0	1	0
3	D	45	0	0	2	0
3	E	39	0	0	6	0
3	F	45	0	0	3	0
All	All	10121	0	9611	56	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 (56) 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:E:138[B]:VAL:HG22	1:E:199[B]:LEU:HD12	1.41	1.01
1:C:75:GLN:HE22	1:D:237:TRP:CD1	1.87	0.92
1:E:138[B]:VAL:CG2	1:E:199[B]:LEU:HD12	2.06	0.85
1:E:188:ARG:NH1	3:E:401:HOH:O	2.24	0.69
1:B:214:THR:HG22	3:B:408:HOH:O	1.96	0.66
1:A:114:LEU:HD12	1:C:129:ARG:HD2	1.80	0.62
1:E:95:GLN:HG2	3:E:436:HOH:O	2.00	0.61
1:C:75:GLN:HE22	1:D:237:TRP:HD1	1.47	0.59
1:A:188:ARG:NH1	1:B:85:VAL:O	2.35	0.59
1:B:86:LEU:HD13	1:B:109:SER:HA	1.84	0.59
1:F:20:ARG:NH1	3:F:402:HOH:O	2.37	0.58
1:F:109:SER:HB2	3:F:439:HOH:O	2.07	0.54
1:A:164:ASP:HB2	3:A:410:HOH:O	2.08	0.53
1:C:75:GLN:HE22	1:D:237:TRP:NE1	2.04	0.53
1:F:87:ARG:HD2	1:F:89:VAL:HG22	1.91	0.53
1:B:124:PRO:HG3	1:D:208:VAL:CG2	2.39	0.52
1:C:109:SER:HB2	3:C:429:HOH:O	2.09	0.52
1:B:124:PRO:HG3	1:D:208:VAL:HG21	1.92	0.51
2:D:301:E85:C22	2:D:301:E85:N10	2.71	0.51
1:E:146:HIS:HD2	3:E:403:HOH:O	1.95	0.49
1:E:87:ARG:HD2	1:E:89:VAL:HG22	1.94	0.48
1:D:147:ALA:HB1	3:D:410:HOH:O	2.13	0.48
1:C:87:ARG:HD2	1:C:89:VAL:HG22	1.96	0.47
1:B:87:ARG:HD2	1:B:89:VAL:HG22	1.95	0.47
1:B:161:PRO:HB2	3:B:402:HOH:O	2.14	0.47
2:C:301:E85:N3	2:C:301:E85:C36	2.77	0.47
1:A:121:ARG:HG2	3:A:450:HOH:O	2.15	0.46
1:E:138[B]:VAL:HG22	1:E:199[B]:LEU:CD1	2.30	0.46
1:F:110:GLU:HG2	3:F:439:HOH:O	2.16	0.46
1:A:87:ARG:HD2	1:A:89:VAL:HG22	1.97	0.46
1:D:87:ARG:HD2	1:D:89:VAL:HG22	1.98	0.46
1:E:146:HIS:CD2	3:E:403:HOH:O	2.69	0.46
1:E:214:THR:HG22	3:E:428:HOH:O	2.16	0.46
1:E:25:HIS:HA	3:E:421:HOH:O	2.17	0.45
1:A:122:PRO:HG2	1:C:127:VAL:HG21	1.98	0.44
1:D:63:LYS:O	1:D:63:LYS:HG3	2.17	0.44
2:A:301:E85:N10	2:A:301:E85:C22	2.80	0.44
1:A:189:ASP:OD2	2:A:301:E85:N41	2.51	0.44
1:F:99:ILE:CD1	1:F:99:ILE:C	2.90	0.44
1:C:86:LEU:HD13	1:C:109:SER:HA	2.01	0.43
1:A:129:ARG:HD2	1:C:114:LEU:HD12	2.01	0.42
1:E:86:LEU:HD13	1:E:109:SER:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ARG:NE	1:F:49:GLU:OE1	2.46	0.42
1:A:86:LEU:HD13	1:A:109[B]:SER:HA	2.02	0.41
1:D:197:GLY:HA3	3:D:420:HOH:O	2.20	0.41
1:A:86:LEU:HD13	1:A:109[A]:SER:HA	2.02	0.41
1:C:75:GLN:NE2	1:D:237:TRP:CD1	2.70	0.41
1:C:75:GLN:CD	1:D:237:TRP:HE1	2.27	0.41
1:C:190:SER:O	2:C:301:E85:N41	2.53	0.41
1:A:161:PRO:HG3	1:B:87:ARG:HG3	2.01	0.41
1:C:189:ASP:OD2	2:C:301:E85:N41	2.54	0.41
1:D:190:SER:O	2:D:301:E85:N41	2.55	0.40
1:D:86:LEU:HD13	1:D:109:SER:HA	2.03	0.40
2:F:301:E85:N10	2:F:301:E85:C15	2.83	0.40
2:F:301:E85:N3	2:F:301:E85:C36	2.85	0.40
2:E:301:E85:N10	2:E:301:E85:C22	2.85	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	210/232 (90%)	206 (98%)	4 (2%)	0	100	100
1	B	207/232 (89%)	203 (98%)	4 (2%)	0	100	100
1	C	212/232 (91%)	209 (99%)	3 (1%)	0	100	100
1	D	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	E	209/232 (90%)	206 (99%)	3 (1%)	0	100	100
1	F	209/232 (90%)	206 (99%)	3 (1%)	0	100	100
All	All	1256/1392 (90%)	1235 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/183 (94%)	164 (95%)	8 (5%)	23	29
1	B	175/183 (96%)	167 (95%)	8 (5%)	24	30
1	C	171/183 (93%)	163 (95%)	8 (5%)	23	29
1	D	173/183 (94%)	166 (96%)	7 (4%)	28	36
1	E	175/183 (96%)	167 (95%)	8 (5%)	24	30
1	F	173/183 (94%)	168 (97%)	5 (3%)	37	49
All	All	1039/1098 (95%)	995 (96%)	44 (4%)	28	34

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	59	LEU
1	A	86	LEU
1	A	129	ARG
1	A	129(A)	ASP
1	A	163	LEU
1	A	240[A]	SER
1	A	240[B]	SER
1	B	23	GLU
1	B	45	VAL
1	B	59	LEU
1	B	86	LEU
1	B	99	ILE
1	B	163	LEU
1	B	240[A]	SER
1	B	240[B]	SER
1	C	45	VAL
1	C	59	LEU
1	C	86	LEU
1	C	129	ARG
1	C	129(A)	ASP
1	C	163	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	240[A]	SER
1	C	240[B]	SER
1	D	23	GLU
1	D	45	VAL
1	D	59	LEU
1	D	63	LYS
1	D	86	LEU
1	D	163	LEU
1	D	224	LYS
1	E	23	GLU
1	E	45	VAL
1	E	59	LEU
1	E	86	LEU
1	E	150	ARG
1	E	163	LEU
1	E	187	ARG
1	E	224	LYS
1	F	45	VAL
1	F	59	LEU
1	F	86	LEU
1	F	99	ILE
1	F	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	B	34	GLN
1	B	95	GLN
1	D	75	GLN
1	D	186	ASN
1	F	75	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	E85	F	301	-	29,29,29	1.20	2 (6%)	33,40,40	2.19	7 (21%)
2	E85	D	301	-	29,29,29	1.14	3 (10%)	33,40,40	2.24	9 (27%)
2	E85	B	301	-	29,29,29	1.09	2 (6%)	33,40,40	2.45	9 (27%)
2	E85	C	301	-	29,29,29	1.05	2 (6%)	33,40,40	2.21	10 (30%)
2	E85	E	301	-	29,29,29	0.91	0	33,40,40	2.19	10 (30%)
2	E85	A	301	-	29,29,29	1.17	2 (6%)	33,40,40	1.97	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E85	F	301	-	-	3/10/10/10	0/4/4/4
2	E85	D	301	-	-	3/10/10/10	0/4/4/4
2	E85	B	301	-	-	1/10/10/10	0/4/4/4
2	E85	C	301	-	-	1/10/10/10	0/4/4/4
2	E85	E	301	-	-	1/10/10/10	0/4/4/4
2	E85	A	301	-	-	0/10/10/10	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	E85	C4-N3	3.90	1.36	1.32
2	A	301	E85	C4-N3	3.89	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	E85	C6-N1	-3.04	1.33	1.35
2	D	301	E85	C4-N3	3.01	1.35	1.32
2	D	301	E85	C22-C14	2.74	1.43	1.39
2	A	301	E85	C28-N26	-2.54	1.36	1.41
2	B	301	E85	C36-C28	2.53	1.43	1.39
2	F	301	E85	C4-N26	2.32	1.40	1.36
2	C	301	E85	C4-N3	2.21	1.34	1.32
2	B	301	E85	C22-C14	2.11	1.42	1.39
2	D	301	E85	C36-C28	2.01	1.42	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	E85	N1-C6-N7	6.52	131.56	125.83
2	B	301	E85	C5-C6-N7	-6.11	120.13	126.64
2	D	301	E85	N7-C8-N10	-6.03	119.46	128.58
2	B	301	E85	N7-C8-N10	-5.93	119.61	128.58
2	F	301	E85	N1-C6-N7	5.72	130.87	125.83
2	A	301	E85	C5-C6-N7	-5.72	120.55	126.64
2	C	301	E85	N7-C8-N10	-5.63	120.05	128.58
2	D	301	E85	N1-C6-N7	5.57	130.73	125.83
2	F	301	E85	N7-C8-N10	-5.51	120.25	128.58
2	D	301	E85	C5-C6-N7	-5.46	120.82	126.64
2	E	301	E85	N7-C8-N10	-5.17	120.75	128.58
2	F	301	E85	C5-C6-N7	-5.03	121.28	126.64
2	C	301	E85	C5-C6-N7	-5.00	121.31	126.64
2	E	301	E85	N1-C6-N7	5.00	130.23	125.83
2	C	301	E85	N1-C6-N7	4.90	130.14	125.83
2	A	301	E85	N7-C8-N10	-4.83	121.27	128.58
2	A	301	E85	N1-C6-N7	4.82	130.07	125.83
2	E	301	E85	C5-C6-N7	-4.68	121.65	126.64
2	C	301	E85	C6-N1-N3	4.49	113.66	111.18
2	B	301	E85	C6-N1-N3	4.39	113.61	111.18
2	E	301	E85	C6-N1-N3	4.04	113.42	111.18
2	F	301	E85	C14-N12-C11	-3.76	120.20	129.43
2	D	301	E85	C14-N12-C11	-3.67	120.43	129.43
2	E	301	E85	C36-C28-C29	-3.13	115.87	119.66
2	D	301	E85	C6-N1-N3	3.13	112.91	111.18
2	F	301	E85	C36-C28-C29	-2.83	116.24	119.66
2	E	301	E85	C14-C15-C17	2.81	121.94	119.56
2	E	301	E85	C5-C11-N10	-2.74	116.18	120.91
2	E	301	E85	C8-N10-C11	2.72	124.24	115.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	E85	C36-C28-C29	-2.70	116.39	119.66
2	B	301	E85	C36-C28-N26	2.66	129.33	120.41
2	E	301	E85	C22-C14-C15	-2.63	116.48	119.66
2	F	301	E85	C8-N10-C11	2.59	123.84	115.24
2	A	301	E85	C5-C6-N1	2.57	109.38	107.58
2	D	301	E85	C8-N10-C11	2.50	123.52	115.24
2	C	301	E85	C28-N26-C4	-2.48	123.26	128.24
2	B	301	E85	C28-C29-C31	2.45	124.05	120.87
2	C	301	E85	C8-N10-C11	2.44	123.34	115.24
2	B	301	E85	C8-N10-C11	2.41	123.22	115.24
2	C	301	E85	C14-C15-C17	2.39	121.58	119.56
2	E	301	E85	C36-C28-N26	2.30	128.13	120.41
2	F	301	E85	C5-C11-N10	-2.24	117.06	120.91
2	D	301	E85	C22-C14-C15	-2.22	116.97	119.66
2	C	301	E85	C22-C14-N12	2.20	128.06	120.61
2	A	301	E85	C8-N10-C11	2.20	122.53	115.24
2	C	301	E85	N12-C11-N10	2.17	121.01	118.38
2	A	301	E85	C14-C15-C17	2.15	121.38	119.56
2	A	301	E85	C28-C29-C31	2.12	123.62	120.87
2	B	301	E85	C14-C15-C17	2.11	121.34	119.56
2	D	301	E85	C14-C15-C17	2.09	121.33	119.56
2	C	301	E85	C5-C11-N10	-2.07	117.34	120.91
2	D	301	E85	C36-C28-C29	-2.07	117.15	119.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

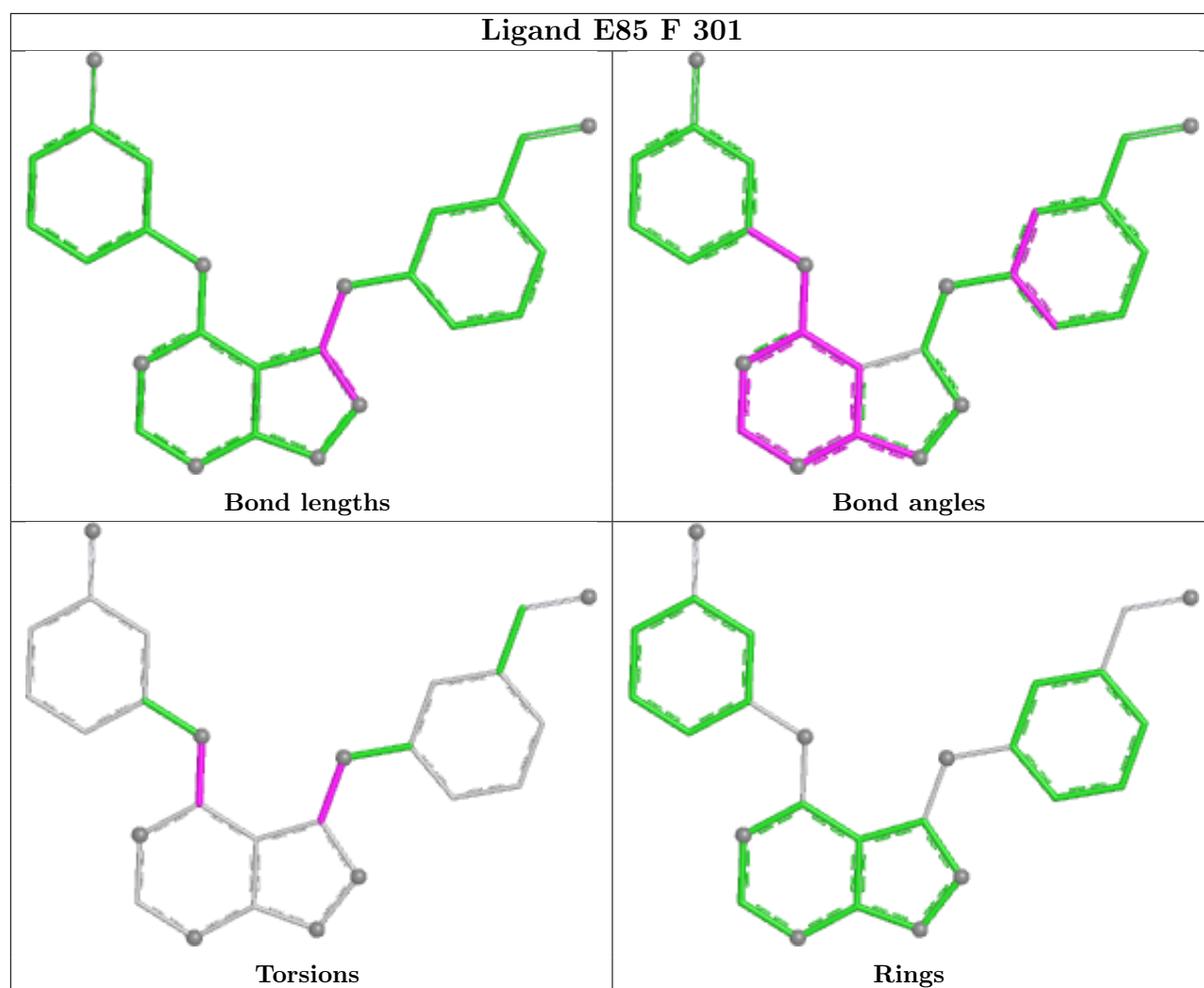
Mol	Chain	Res	Type	Atoms
2	B	301	E85	C5-C4-N26-C28
2	C	301	E85	C5-C4-N26-C28
2	D	301	E85	C5-C11-N12-C14
2	E	301	E85	C5-C4-N26-C28
2	F	301	E85	C5-C4-N26-C28
2	F	301	E85	C5-C11-N12-C14
2	F	301	E85	N10-C11-N12-C14
2	D	301	E85	N10-C11-N12-C14
2	D	301	E85	C32-C31-C38-N41

There are no ring outliers.

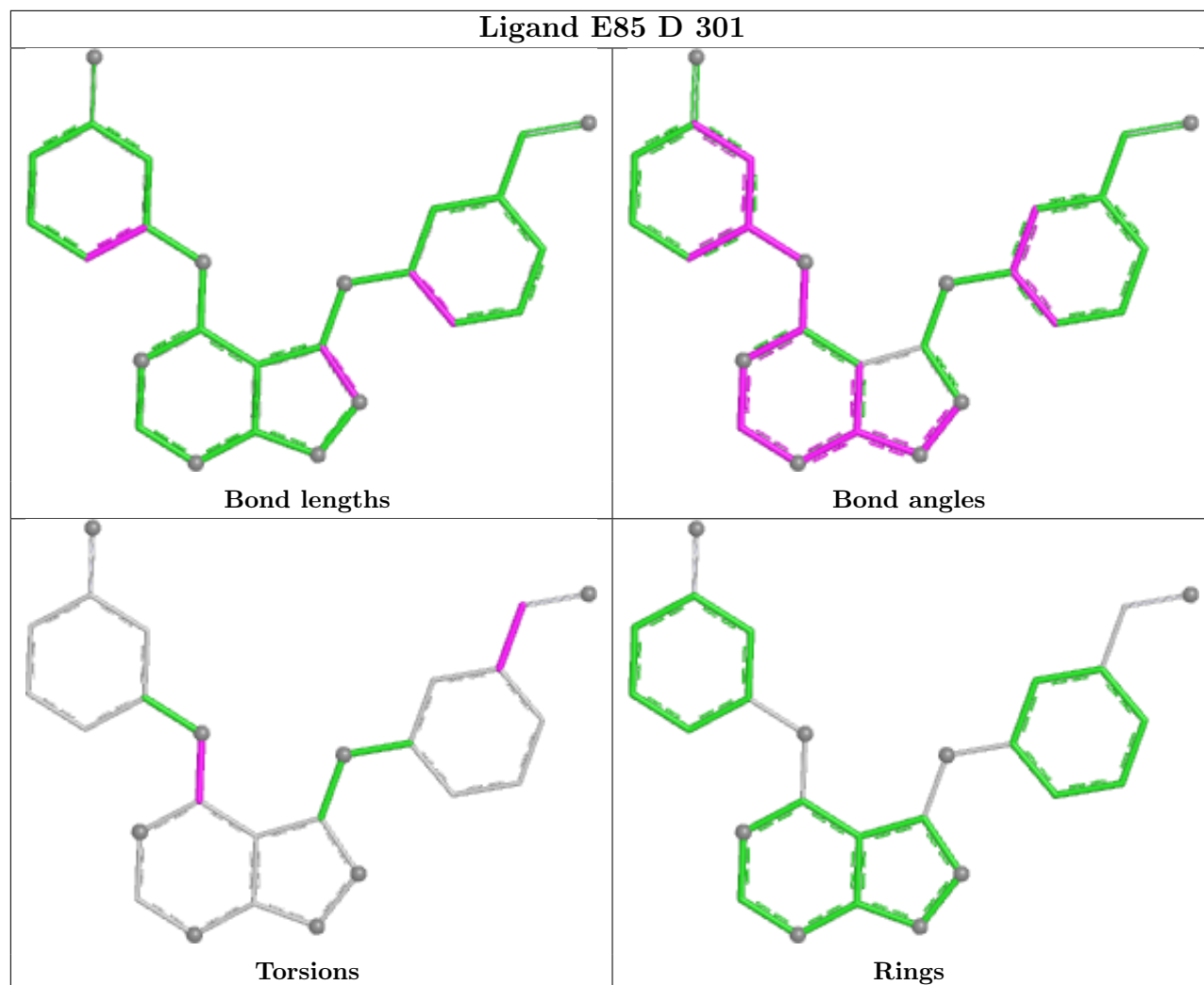
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	E85	2	0
2	D	301	E85	2	0
2	C	301	E85	3	0
2	E	301	E85	1	0
2	A	301	E85	2	0

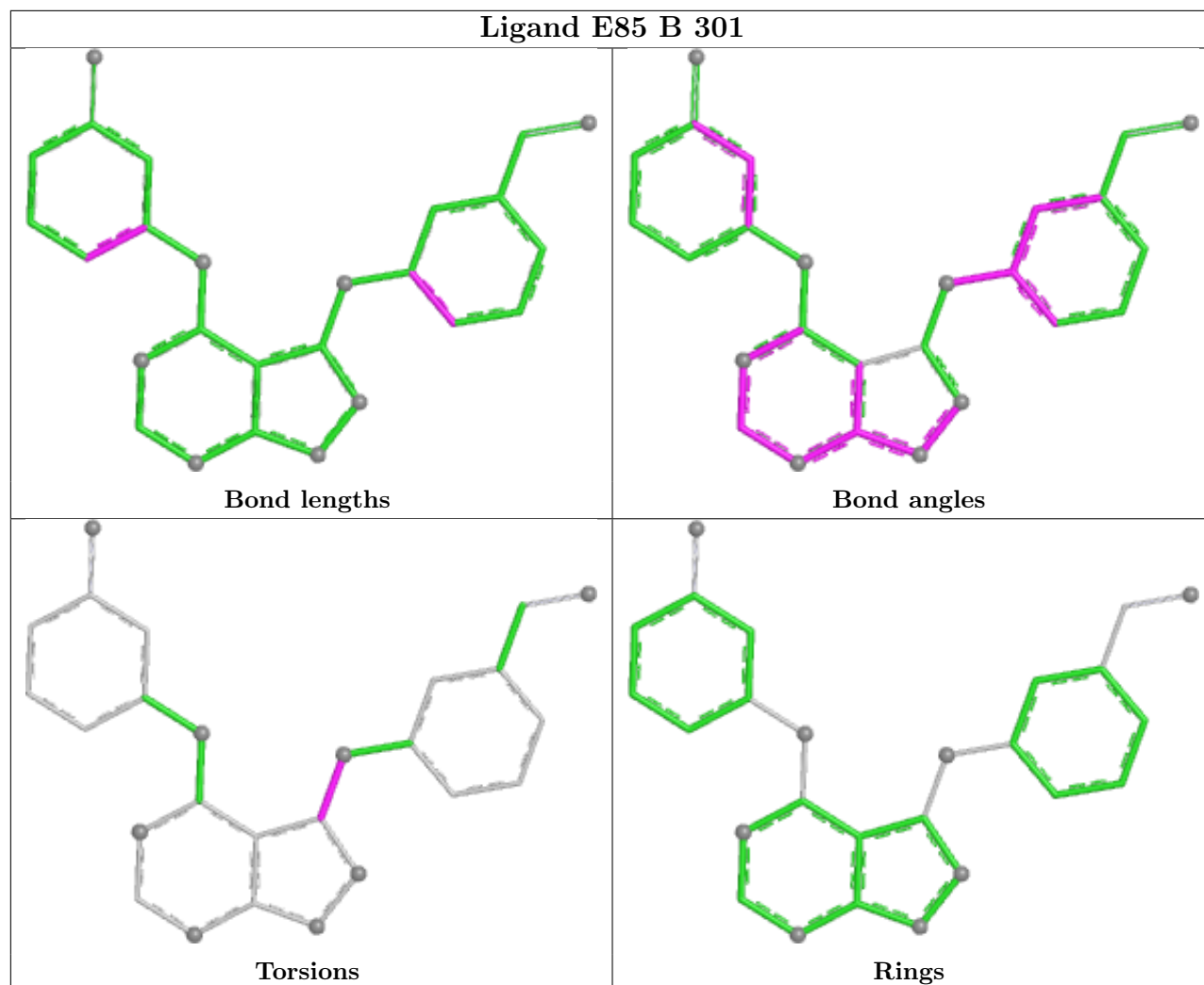
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



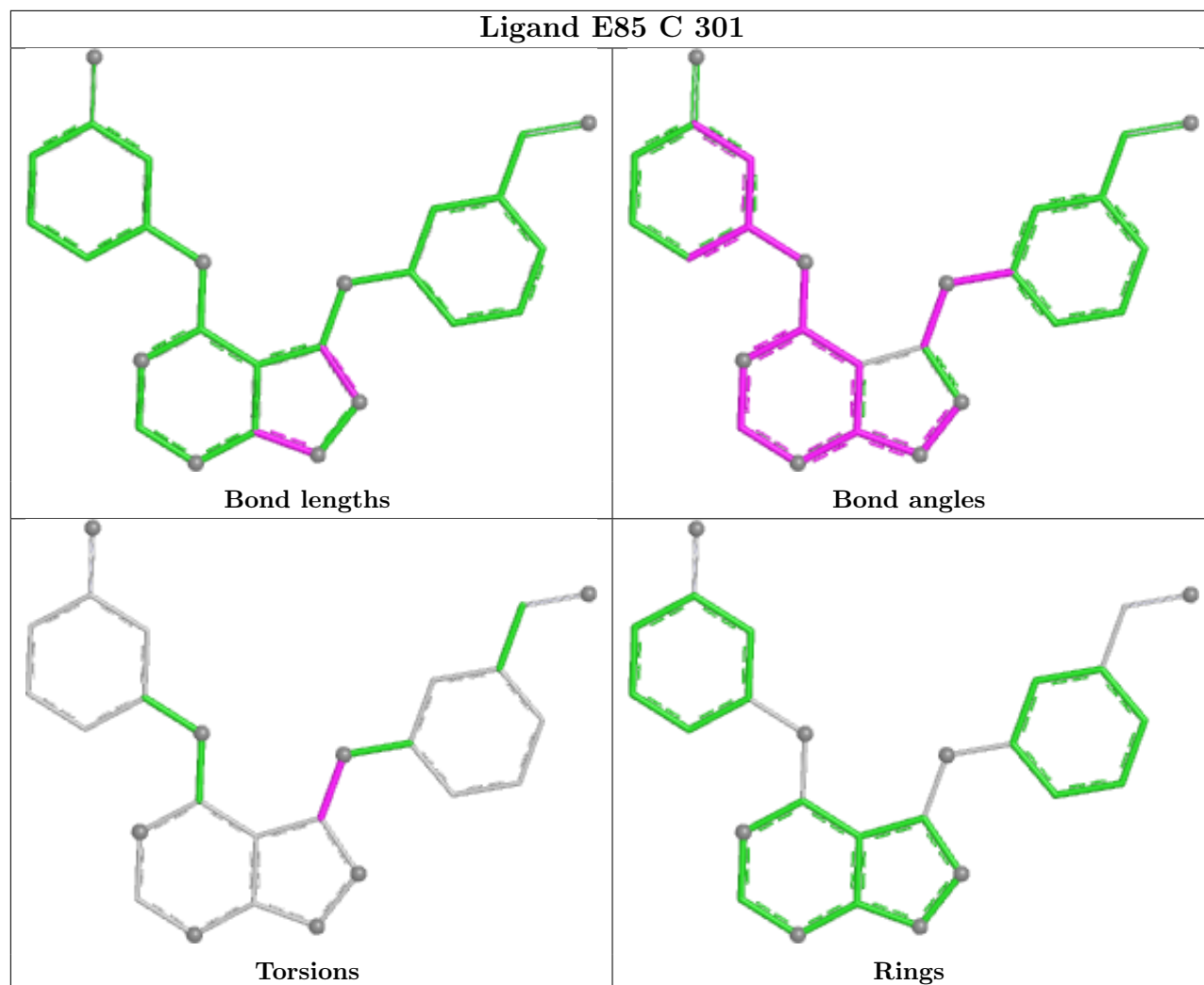
Ligand E85 D 301

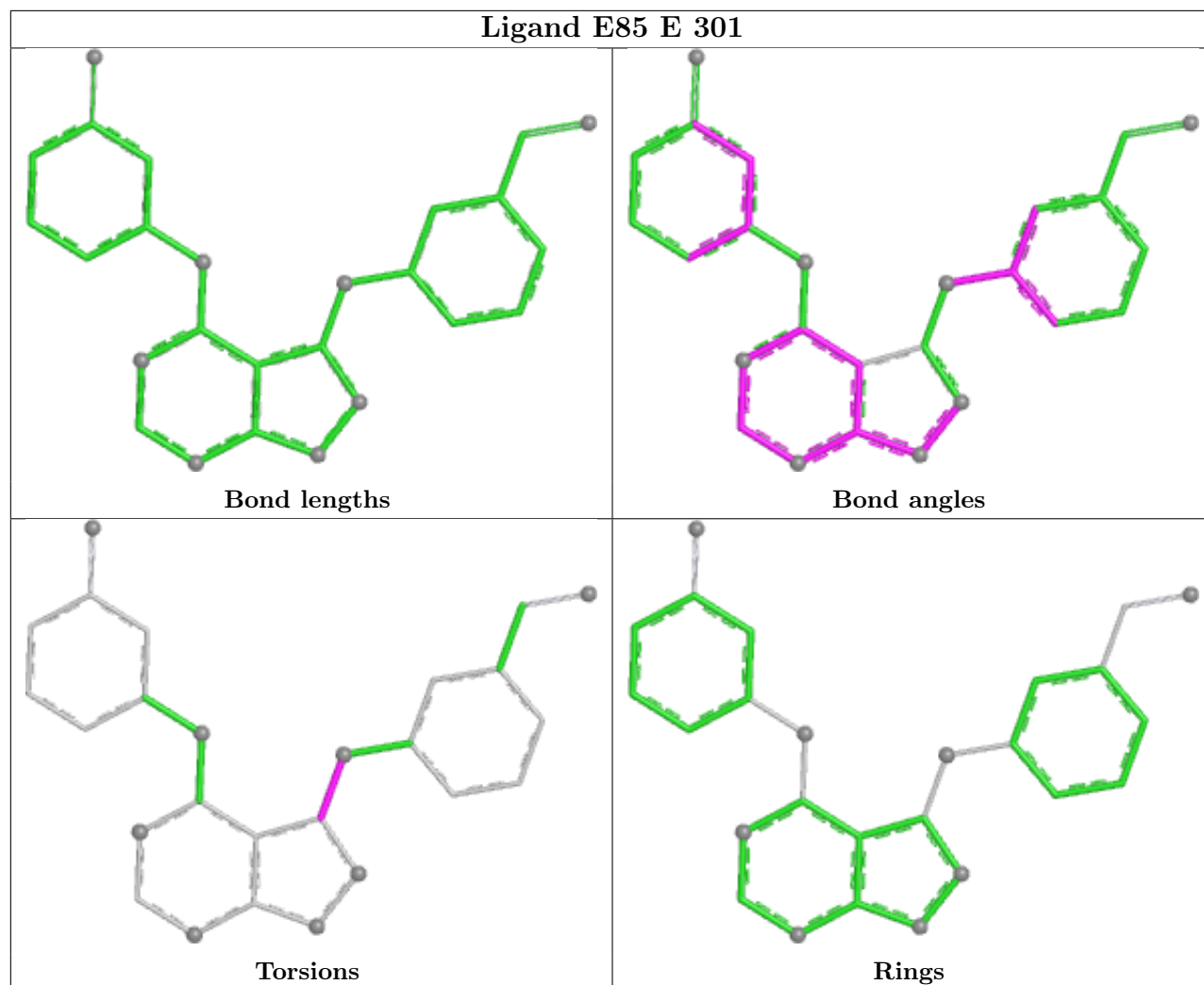


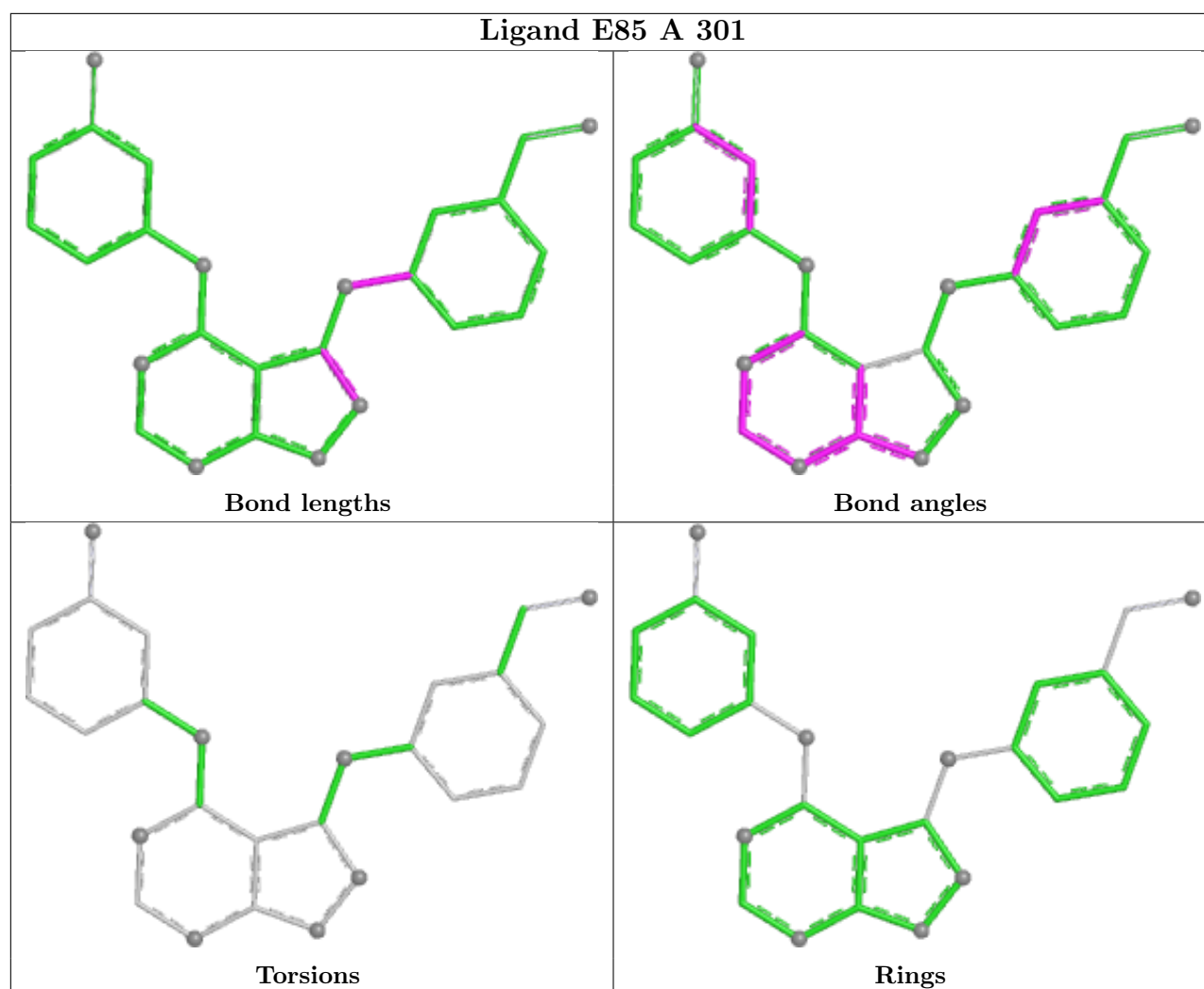
Ligand E85 B 301



Ligand E85 C 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	169:ASN	C	173:ARG	N	4.85

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/232 (93%)	0.12	4 (1%) 66 64	18, 32, 54, 80	2 (0%)
1	B	211/232 (90%)	0.39	9 (4%) 40 37	14, 37, 70, 85	6 (2%)
1	C	218/232 (93%)	0.61	13 (5%) 27 25	21, 45, 70, 133	2 (0%)
1	D	214/232 (92%)	0.49	9 (4%) 40 37	15, 40, 65, 87	3 (1%)
1	E	213/232 (91%)	0.55	18 (8%) 16 14	12, 42, 75, 100	4 (1%)
1	F	213/232 (91%)	0.59	10 (4%) 36 33	12, 44, 75, 103	4 (1%)
All	All	1285/1392 (92%)	0.46	63 (4%) 35 31	12, 40, 70, 133	21 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	SER	3.5
1	B	97	ASP	3.5
1	D	62	GLY	3.5
1	C	97	ASP	3.5
1	B	221	GLY	3.4
1	B	76	PRO	3.4
1	B	62	GLY	3.3
1	E	35	LEU	3.3
1	E	62	GLY	3.2
1	E	57	HIS	3.2
1	A	245	ALA	3.1
1	F	57	HIS	3.0
1	A	244	SER	2.8
1	C	243	ALA	2.7
1	D	245	ALA	2.7
1	E	108	LEU	2.7
1	C	245	ALA	2.7
1	E	245	ALA	2.7
1	A	243	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	219	VAL	2.6
1	C	98	THR	2.6
1	B	145	ASN	2.6
1	E	23	GLU	2.6
1	C	62	GLY	2.6
1	B	218	ARG	2.5
1	D	57	HIS	2.5
1	D	76	PRO	2.5
1	F	245	ALA	2.5
1	D	218	ARG	2.4
1	D	152	PRO	2.4
1	E	76	PRO	2.4
1	D	214	THR	2.4
1	B	23	GLU	2.3
1	C	175	ALA	2.3
1	C	144	VAL	2.3
1	F	59	LEU	2.3
1	C	173	ARG	2.3
1	E	58	CYS	2.3
1	E	88	ALA	2.3
1	E	82	LEU	2.2
1	F	164	ASP	2.2
1	B	57	HIS	2.2
1	F	149	GLY	2.2
1	D	60	GLU	2.2
1	A	214	THR	2.2
1	C	244	SER	2.2
1	C	59	LEU	2.2
1	E	164	ASP	2.2
1	E	38	GLY	2.2
1	F	99	ILE	2.2
1	E	79	SER	2.2
1	E	166	ALA	2.2
1	E	244	SER	2.2
1	C	99	ILE	2.1
1	D	222	ASN	2.1
1	C	220	CYS	2.1
1	F	81	ARG	2.1
1	E	224	LYS	2.0
1	C	109	SER	2.0
1	F	35	LEU	2.0
1	F	98	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	244	SER	2.0
1	B	243	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

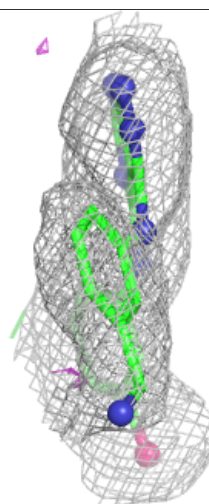
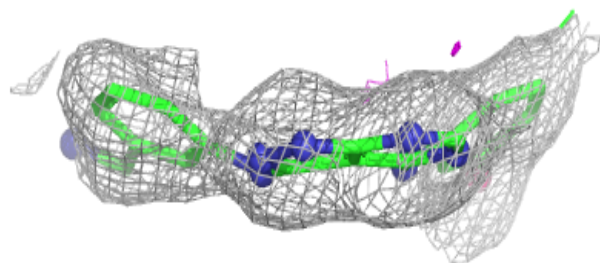
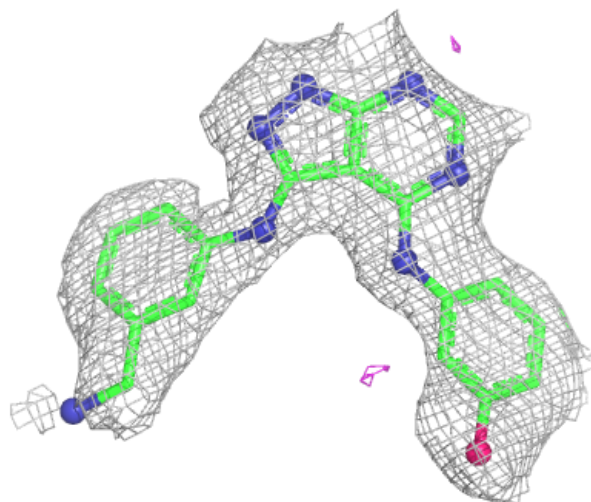
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	E85	B	301	26/26	0.83	0.11	44,54,59,62	0
2	E85	E	301	26/26	0.85	0.10	44,52,61,63	0
2	E85	F	301	26/26	0.85	0.10	36,48,61,65	0
2	E85	C	301	26/26	0.86	0.10	50,55,61,67	0
2	E85	D	301	26/26	0.86	0.10	42,52,65,69	0
2	E85	A	301	26/26	0.94	0.07	26,31,45,46	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.

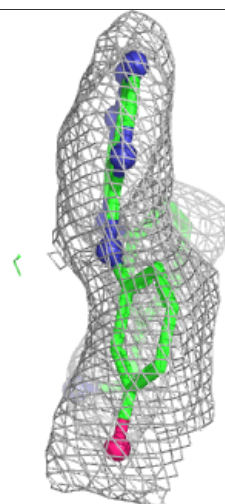
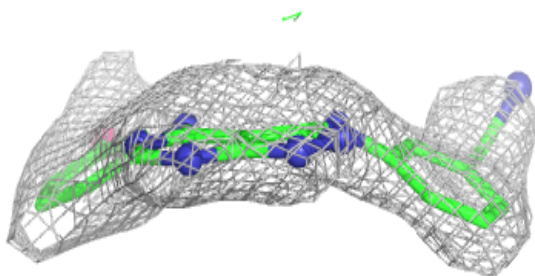
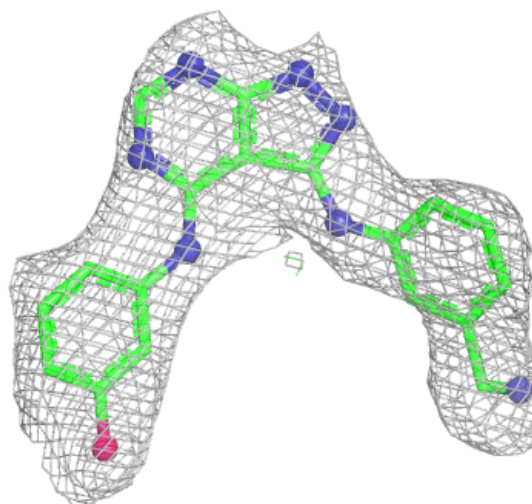
Electron density around E85 B 301:

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



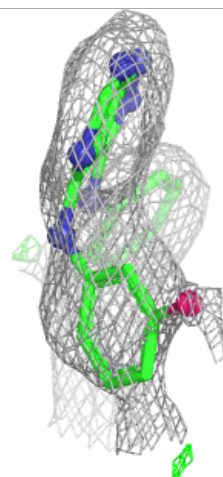
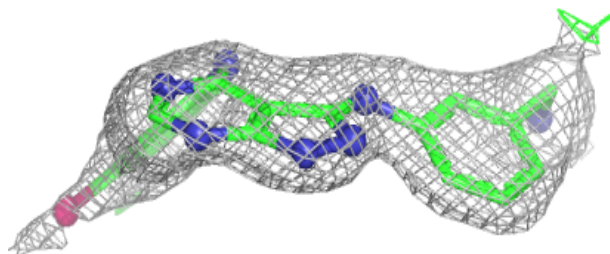
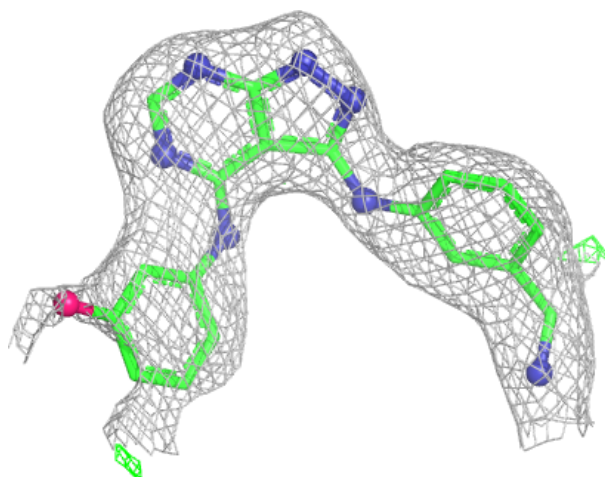
Electron density around E85 E 301:

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



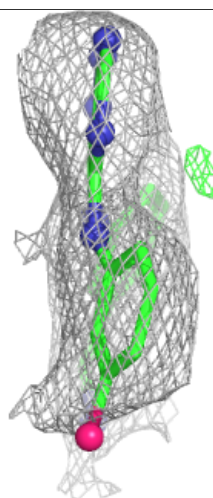
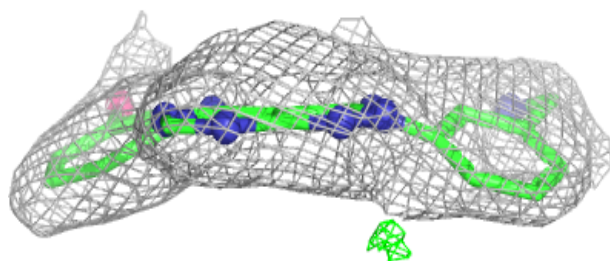
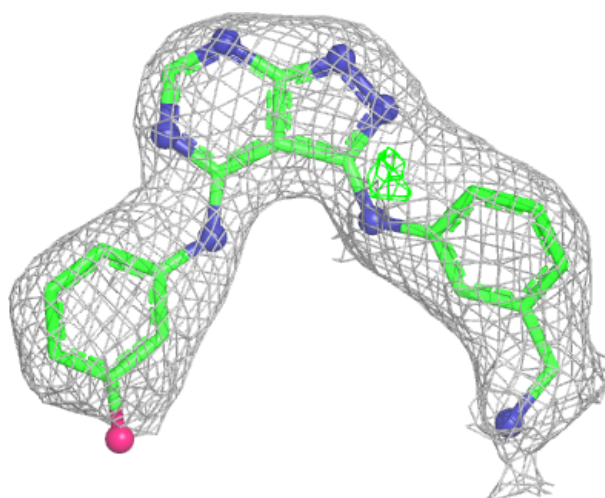
Electron density around E85 F 301:

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



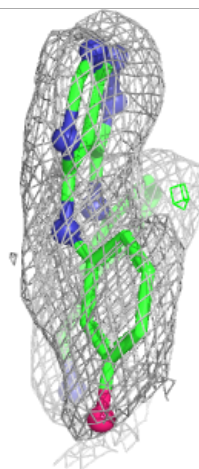
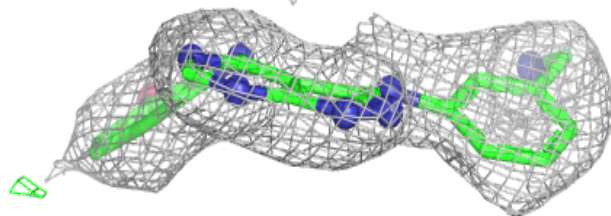
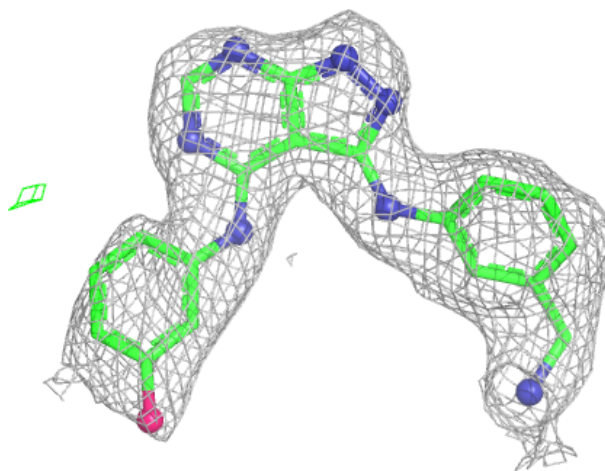
Electron density around E85 C 301:

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



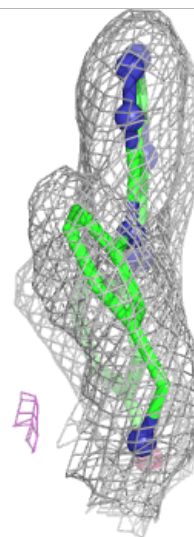
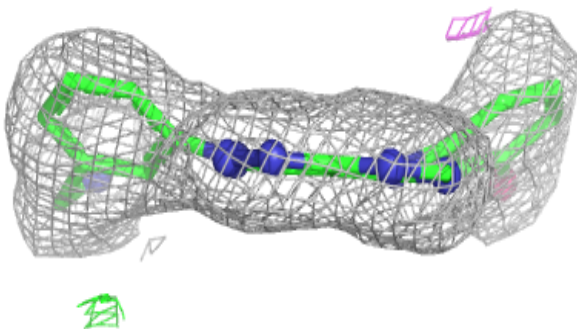
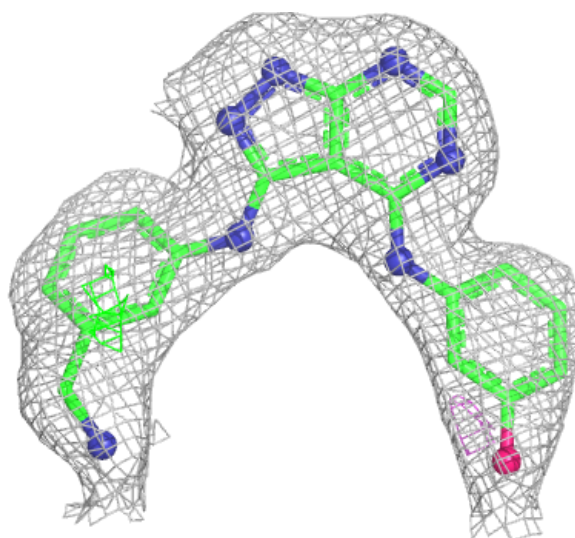
Electron density around E85 D 301:

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



Electron density around E85 A 301:

$2mF_o-DF_c$ (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.