



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:35 PM UTC

PDB ID : 8P22 / pdb_00008p22
Title : X-ray structure of acetylcholine-binding protein (AChBP) in complex with IOTA376.
Authors : Cederfelt, D.; Boronat, P.; Dobritsch, D.; Hennig, S.; Fitzgerald, E.A.; de Esch, I.J.P.; Danielson, U.H.
Deposited on : 2023-05-14
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

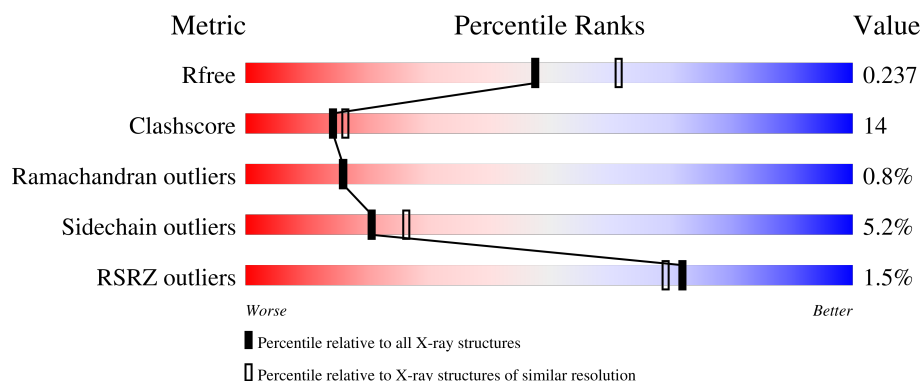
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	206	68% 27% ..
1	B	206	66% 29% ..
1	C	206	3% 65% 29% ..
1	D	206	2% 74% 21% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	206	
1	F	206	
1	G	206	
1	H	206	
1	I	206	
1	J	206	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	302	-	-	X	-
3	SO4	C	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17025 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1600	1006	274	315	5			
1	B	199	Total	C	N	O	S	0	0	0
			1596	1004	273	314	5			
1	C	201	Total	C	N	O	S	0	0	0
			1609	1011	275	318	5			
1	D	201	Total	C	N	O	S	0	0	0
			1609	1011	275	318	5			
1	E	200	Total	C	N	O	S	0	0	0
			1605	1009	274	317	5			
1	F	200	Total	C	N	O	S	0	0	0
			1600	1006	274	315	5			
1	G	198	Total	C	N	O	S	0	0	0
			1589	1000	272	312	5			
1	H	199	Total	C	N	O	S	0	0	0
			1593	1002	273	313	5			
1	I	201	Total	C	N	O	S	0	0	0
			1611	1012	278	316	5			
1	J	199	Total	C	N	O	S	0	0	0
			1596	1004	273	314	5			

There are 20 discrepancies between the modelled and reference sequences:

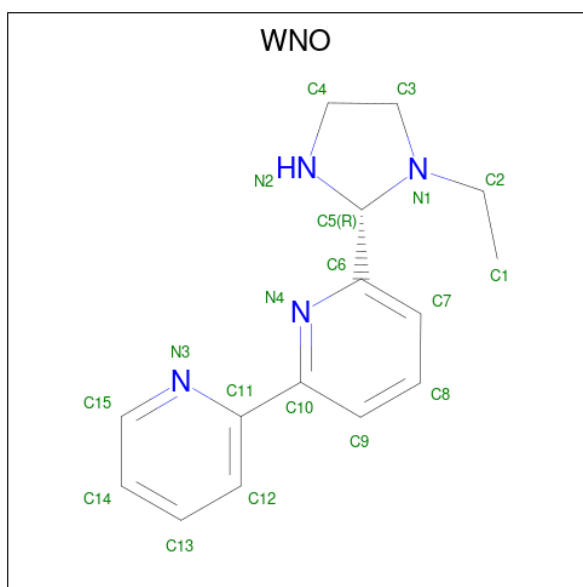
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	PHE	LEU	conflict	UNP P58154
A	225	ARG	-	expression tag	UNP P58154
B	20	PHE	LEU	conflict	UNP P58154
B	225	ARG	-	expression tag	UNP P58154
C	20	PHE	LEU	conflict	UNP P58154
C	225	ARG	-	expression tag	UNP P58154
D	20	PHE	LEU	conflict	UNP P58154
D	225	ARG	-	expression tag	UNP P58154
E	20	PHE	LEU	conflict	UNP P58154

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	225	ARG	-	expression tag	UNP P58154
F	20	PHE	LEU	conflict	UNP P58154
F	225	ARG	-	expression tag	UNP P58154
G	20	PHE	LEU	conflict	UNP P58154
G	225	ARG	-	expression tag	UNP P58154
H	20	PHE	LEU	conflict	UNP P58154
H	225	ARG	-	expression tag	UNP P58154
I	20	PHE	LEU	conflict	UNP P58154
I	225	ARG	-	expression tag	UNP P58154
J	20	PHE	LEU	conflict	UNP P58154
J	225	ARG	-	expression tag	UNP P58154

- Molecule 2 is 2-[(2 {R})-1-ethylimidazolidin-2-yl]-6-pyridin-2-yl-pyridine (CCD ID: WNO) (formula: C₁₅H₁₈N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			19	15	4		
2	C	1	Total	C	N	0	0
			19	15	4		
2	C	1	Total	C	N	0	0
			19	15	4		
2	D	1	Total	C	N	0	0
			19	15	4		
2	E	1	Total	C	N	0	0
			19	15	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	N	0	0
			19	15	4		
2	G	1	Total	C	N	0	0
			19	15	4		
2	H	1	Total	C	N	0	0
			19	15	4		
2	I	1	Total	C	N	0	0
			19	15	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			6	3	3		

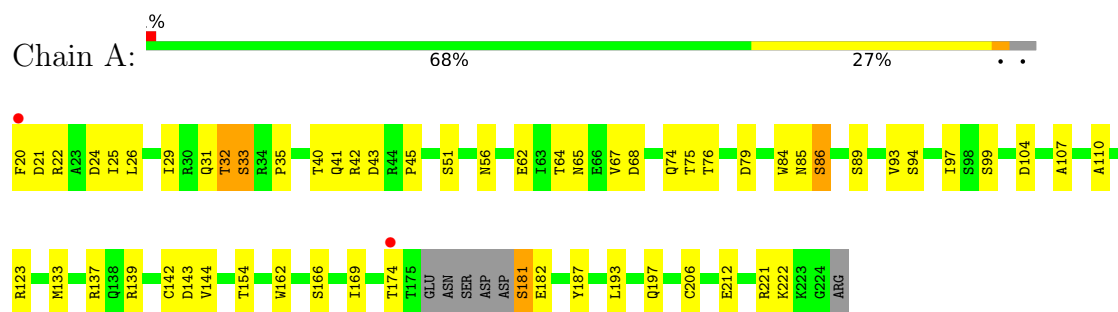
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	78	Total	O	0	0
			78	78		
5	C	84	Total	O	0	0
			84	84		
5	D	86	Total	O	0	0
			86	86		
5	E	83	Total	O	0	0
			83	83		
5	F	78	Total	O	0	0
			78	78		
5	G	100	Total	O	0	0
			100	100		
5	H	72	Total	O	0	0
			72	72		
5	I	64	Total	O	0	0
			64	64		
5	J	93	Total	O	0	0
			93	93		

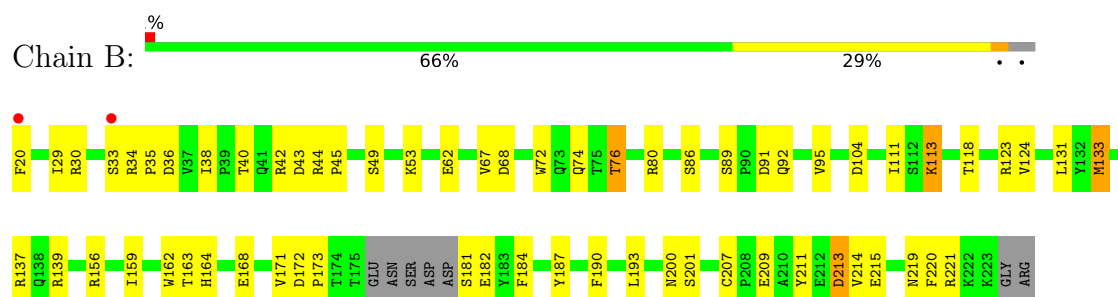
3 Residue-property plots

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.

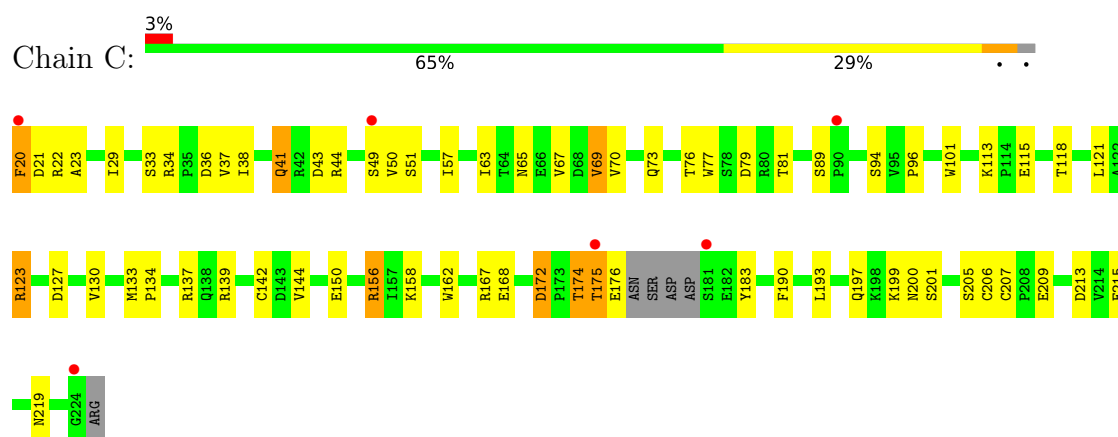
• Molecule 1: Acetylcholine-binding protein



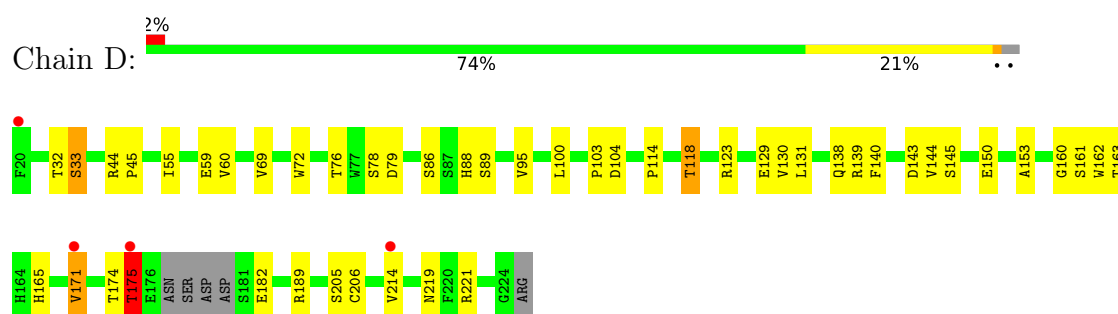
• Molecule 1: Acetylcholine-binding protein



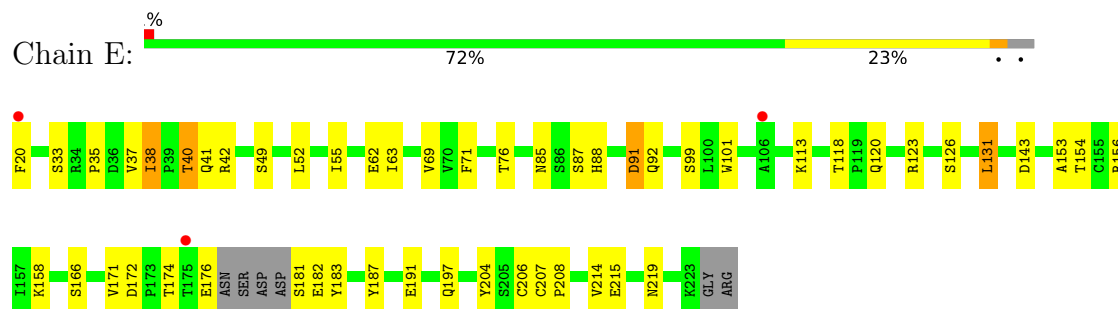
• Molecule 1: Acetylcholine-binding protein



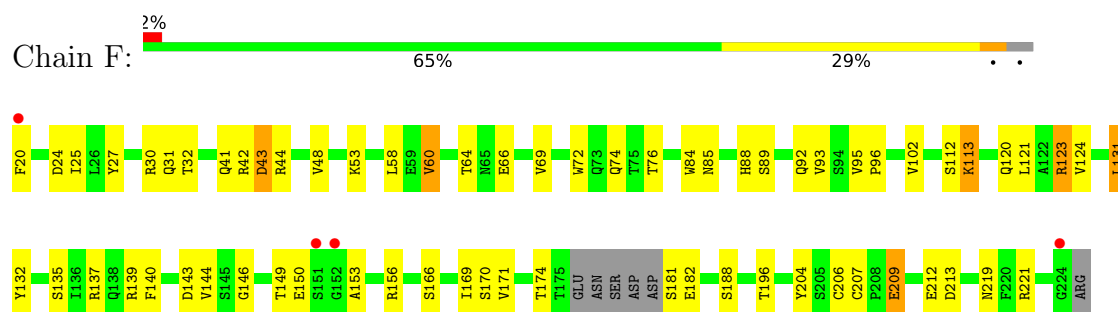
• Molecule 1: Acetylcholine-binding protein



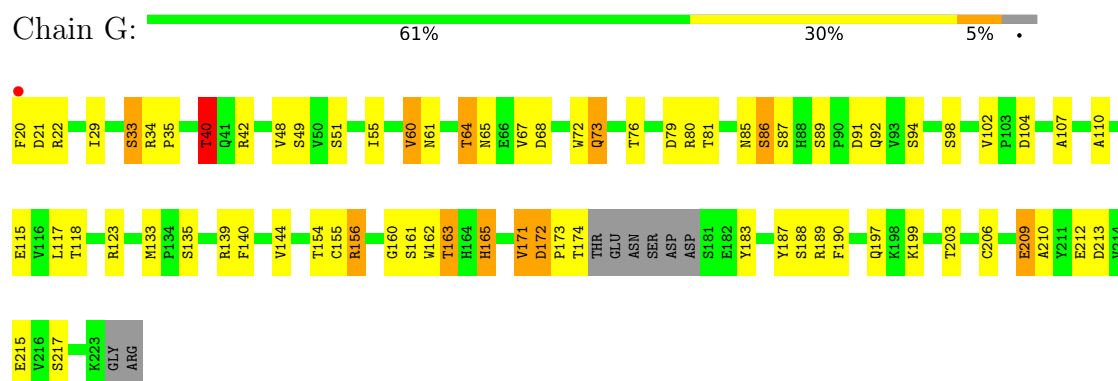
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

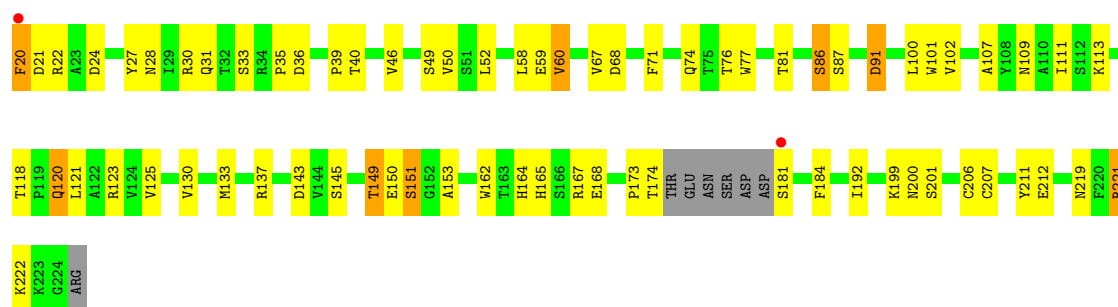


- Molecule 1: Acetylcholine-binding protein

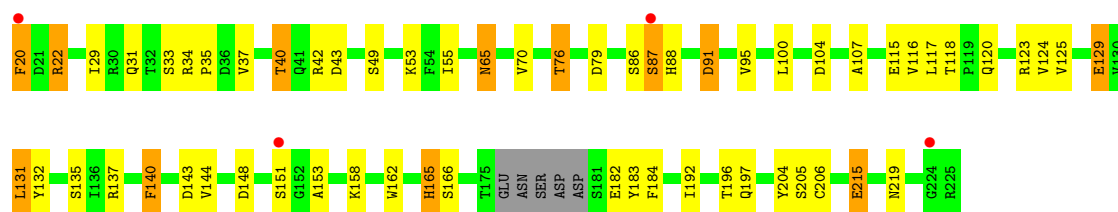


- Molecule 1: Acetylcholine-binding protein

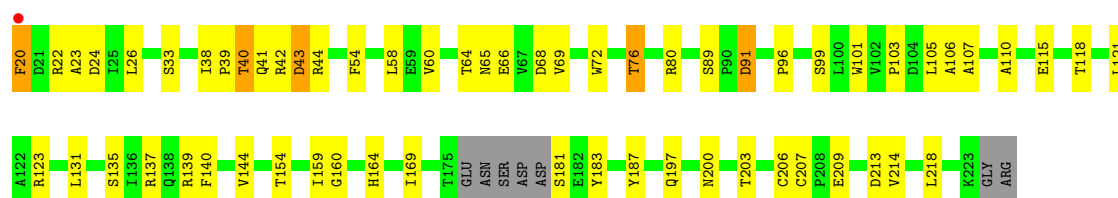




• Molecule 1: Acetylcholine-binding protein



• Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.96Å 120.60Å 133.16Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	49.51 – 2.20 49.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.3 (49.51-2.20) 88.3 (49.51-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.238 , 0.304 0.238 , 0.237	Depositor DCC
R_{free} test set	5090 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17025	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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: WNO, GOL, SO4

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	0.61	0/1636	1.17	4/2231 (0.2%)
1	B	0.63	0/1632	1.20	9/2226 (0.4%)
1	C	0.62	0/1645	1.18	11/2243 (0.5%)
1	D	0.63	0/1645	1.12	1/2243 (0.0%)
1	E	0.62	0/1641	1.20	6/2238 (0.3%)
1	F	0.62	0/1636	1.23	7/2231 (0.3%)
1	G	0.63	0/1625	1.20	7/2216 (0.3%)
1	H	0.62	0/1629	1.23	12/2221 (0.5%)
1	I	0.60	0/1647	1.13	4/2245 (0.2%)
1	J	0.65	1/1632 (0.1%)	1.21	4/2226 (0.2%)
All	All	0.62	1/16368 (0.0%)	1.19	65/22320 (0.3%)

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	B	0	1
1	C	0	4
1	D	0	2
1	G	0	2
1	H	0	3
1	I	0	3
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	39	PRO	CA-CB	-5.19	1.50	1.53

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ARG	N-CA-CB	-11.73	92.16	110.57
1	E	91	ASP	CA-CB-CG	10.14	122.74	112.60
1	H	123	ARG	CB-CA-C	8.19	123.25	109.48
1	F	88	HIS	CB-CA-C	7.14	122.65	111.72
1	H	40	THR	CA-CB-OG1	-7.03	99.06	109.60

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	221	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	156	ARG	Sidechain
1	C	167	ARG	Sidechain
1	C	174	THR	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	1600	0	1550	45	0
1	B	1596	0	1547	45	0
1	C	1609	0	1556	43	0
1	D	1609	0	1556	38	0
1	E	1605	0	1553	38	0
1	F	1600	0	1550	59	0
1	G	1589	0	1540	66	0
1	H	1593	0	1543	49	0
1	I	1611	0	1563	49	0
1	J	1596	0	1547	49	0
2	A	19	0	0	2	0
2	C	38	0	0	3	0
2	D	19	0	0	2	0
2	E	19	0	0	3	0
2	F	19	0	0	2	0
2	G	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	19	0	0	0	0
2	I	19	0	0	0	0
3	A	5	0	0	2	0
3	C	5	0	0	3	0
3	F	5	0	0	1	0
4	J	6	0	8	0	0
5	A	87	0	0	12	0
5	B	78	0	0	10	0
5	C	84	0	0	7	0
5	D	86	0	0	6	0
5	E	83	0	0	12	0
5	F	78	0	0	28	0
5	G	100	0	0	32	0
5	H	72	0	0	24	0
5	I	64	0	0	11	0
5	J	93	0	0	14	0
All	All	17025	0	15513	447	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 14.

The worst 5 of 447 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:F:69:VAL:HG22	5:F:423:HOH:O	1.29	1.24
1:F:92:GLN:HA	5:F:402:HOH:O	1.34	1.24
1:H:35:PRO:HA	5:H:401:HOH:O	1.33	1.23
5:F:406:HOH:O	1:J:206:CYS:SG	1.95	1.21
1:J:106:ALA:O	5:J:401:HOH:O	1.59	1.20

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	196/206 (95%)	186 (95%)	7 (4%)	3 (2%)	8	6
1	B	195/206 (95%)	188 (96%)	6 (3%)	1 (0%)	24	27
1	C	197/206 (96%)	188 (95%)	8 (4%)	1 (0%)	24	27
1	D	197/206 (96%)	184 (93%)	10 (5%)	3 (2%)	8	6
1	E	196/206 (95%)	187 (95%)	8 (4%)	1 (0%)	24	27
1	F	196/206 (95%)	183 (93%)	12 (6%)	1 (0%)	24	27
1	G	194/206 (94%)	186 (96%)	6 (3%)	2 (1%)	12	11
1	H	195/206 (95%)	187 (96%)	7 (4%)	1 (0%)	24	27
1	I	197/206 (96%)	188 (95%)	8 (4%)	1 (0%)	24	27
1	J	195/206 (95%)	188 (96%)	6 (3%)	1 (0%)	24	27
All	All	1958/2060 (95%)	1865 (95%)	78 (4%)	15 (1%)	16	16

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	J	43	ASP
1	F	43	ASP
1	G	86	SER
1	G	165	HIS

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	186/192 (97%)	175 (94%)	11 (6%)	18	22
1	B	186/192 (97%)	182 (98%)	4 (2%)	45	61
1	C	187/192 (97%)	175 (94%)	12 (6%)	16	19
1	D	187/192 (97%)	182 (97%)	5 (3%)	39	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	187/192 (97%)	177 (95%)	10 (5%)	20	26
1	F	186/192 (97%)	178 (96%)	8 (4%)	26	35
1	G	185/192 (96%)	172 (93%)	13 (7%)	14	16
1	H	185/192 (96%)	173 (94%)	12 (6%)	15	18
1	I	187/192 (97%)	174 (93%)	13 (7%)	14	16
1	J	186/192 (97%)	178 (96%)	8 (4%)	26	35
All	All	1862/1920 (97%)	1766 (95%)	96 (5%)	21	26

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	102	VAL
1	H	151	SER
1	G	156	ARG
1	H	67	VAL
1	I	20	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	31	GLN
1	J	65	ASN
1	G	219	ASN
1	J	219	ASN
1	I	138	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 oligosaccharides in this entry.

5.6 Ligand geometry

13 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	WNO	F	301	-	21,21,21	2.99	3 (14%)	26,28,28	2.54	5 (19%)
3	SO4	C	303	-	4,4,4	0.33	0	6,6,6	0.32	0
2	WNO	G	301	-	21,21,21	2.51	3 (14%)	26,28,28	2.26	6 (23%)
2	WNO	E	301	-	21,21,21	2.47	3 (14%)	26,28,28	2.19	6 (23%)
2	WNO	C	301	-	21,21,21	2.59	3 (14%)	26,28,28	2.25	6 (23%)
2	WNO	D	301	-	21,21,21	2.61	3 (14%)	26,28,28	2.31	6 (23%)
3	SO4	A	302	-	4,4,4	0.35	0	6,6,6	0.14	0
4	GOL	J	301	-	5,5,5	0.21	0	5,5,5	0.57	0
2	WNO	H	301	-	21,21,21	2.47	3 (14%)	26,28,28	2.34	9 (34%)
2	WNO	C	302	-	21,21,21	2.44	4 (19%)	26,28,28	2.58	6 (23%)
3	SO4	F	302	-	4,4,4	0.41	0	6,6,6	0.14	0
2	WNO	A	301	-	21,21,21	2.54	3 (14%)	26,28,28	2.21	8 (30%)
2	WNO	I	301	-	21,21,21	2.69	4 (19%)	26,28,28	2.10	6 (23%)

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	WNO	F	301	-	-	4/10/20/20	0/3/3/3
2	WNO	G	301	-	-	1/10/20/20	0/3/3/3
2	WNO	E	301	-	-	3/10/20/20	0/3/3/3
2	WNO	C	301	-	-	3/10/20/20	0/3/3/3
2	WNO	D	301	-	-	1/10/20/20	0/3/3/3
4	GOL	J	301	-	-	4/4/4/4	-
2	WNO	H	301	-	-	7/10/20/20	0/3/3/3
2	WNO	C	302	-	-	5/10/20/20	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WNO	A	301	-	-	5/10/20/20	0/3/3/3
2	WNO	I	301	-	-	5/10/20/20	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	WNO	C3-C4	-11.04	1.33	1.52
2	C	301	WNO	C3-C4	-9.55	1.36	1.52
2	I	301	WNO	C3-C4	-9.29	1.36	1.52
2	D	301	WNO	C3-C4	-9.13	1.36	1.52
2	G	301	WNO	C3-C4	-8.92	1.37	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	WNO	C2-N1-C5	8.74	126.77	114.13
2	F	301	WNO	C2-N1-C5	7.59	125.11	114.13
2	D	301	WNO	C2-N1-C5	7.56	125.07	114.13
2	G	301	WNO	C2-N1-C5	7.13	124.44	114.13
2	E	301	WNO	C2-N1-C5	7.09	124.39	114.13

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	WNO	C1-C2-N1-C3
2	C	301	WNO	C1-C2-N1-C3
2	C	301	WNO	N1-C5-C6-C7
2	C	301	WNO	N1-C5-C6-N4
2	C	302	WNO	C1-C2-N1-C5

There are no ring outliers.

9 monomers are involved in 18 short contacts:

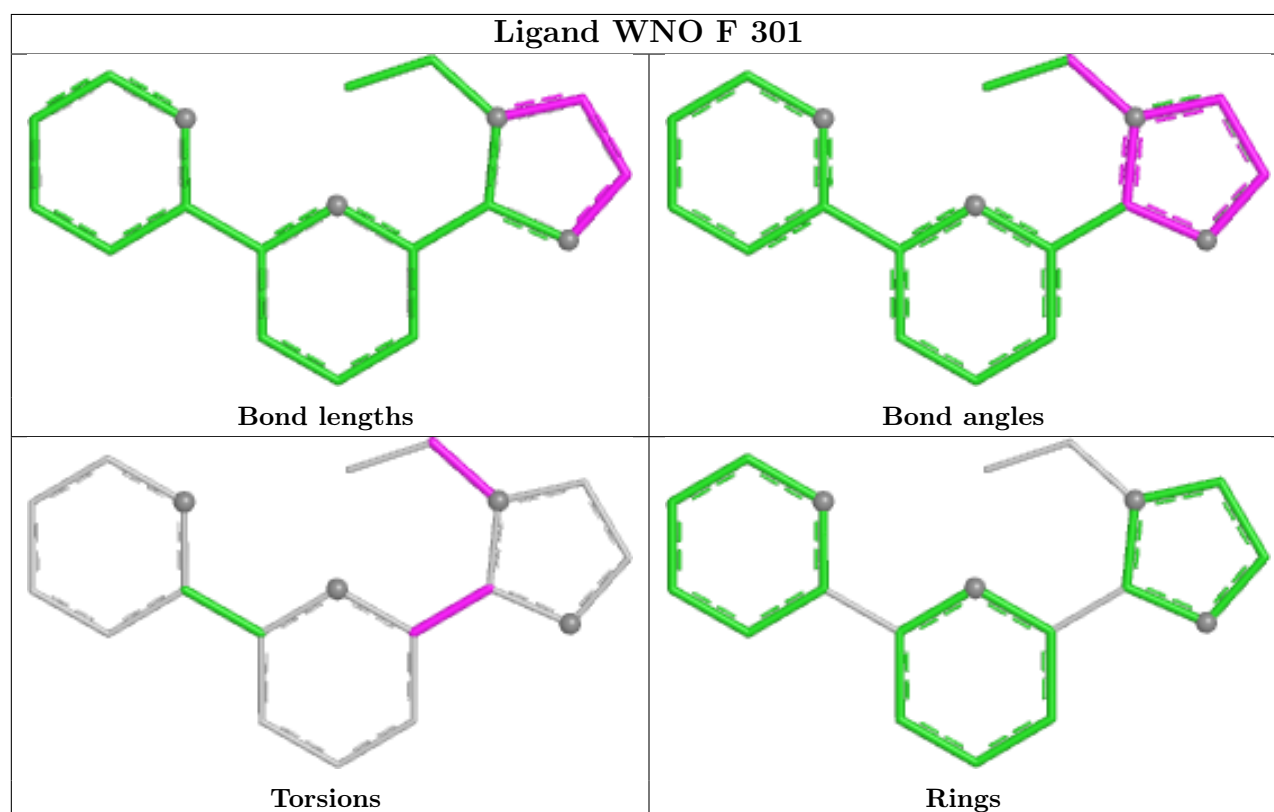
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	WNO	2	0
3	C	303	SO4	3	0
2	E	301	WNO	3	0
2	C	301	WNO	2	0
2	D	301	WNO	2	0

Continued on next page...

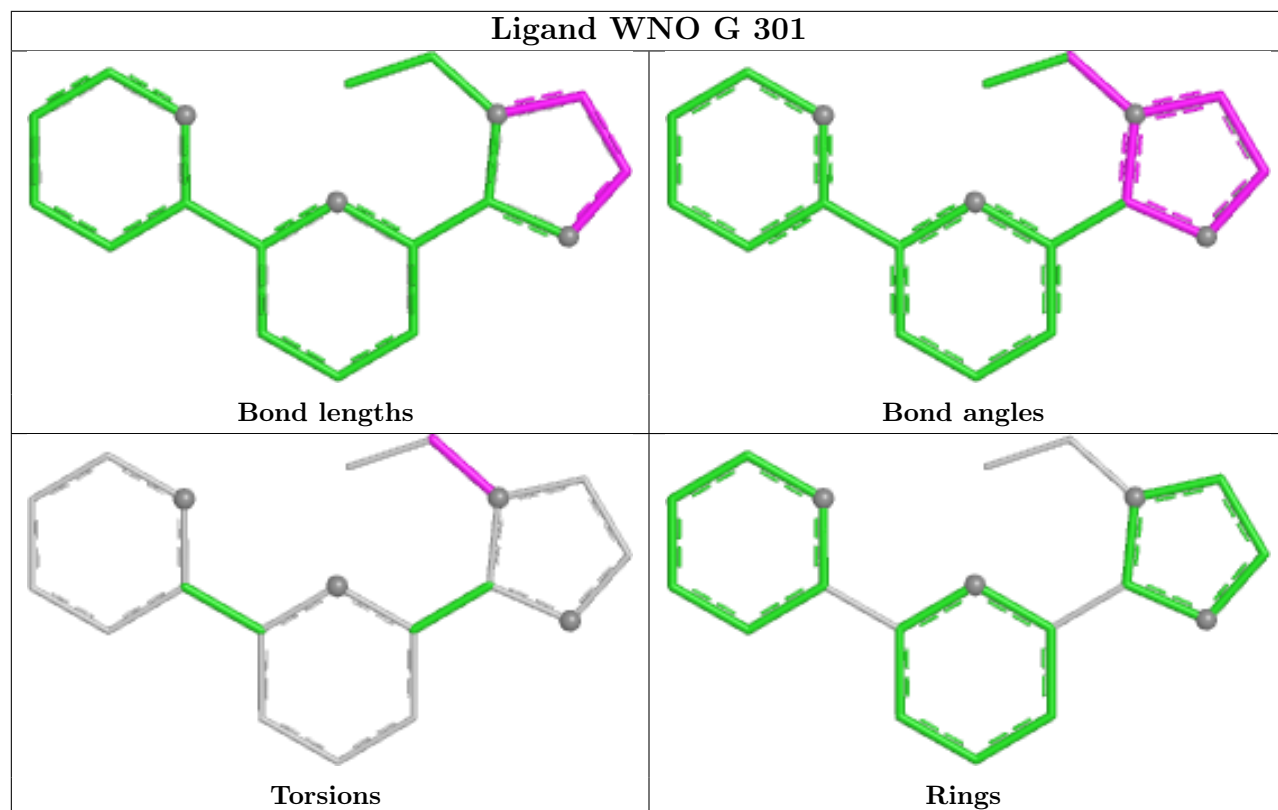
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SO4	2	0
2	C	302	WNO	1	0
3	F	302	SO4	1	0
2	A	301	WNO	2	0

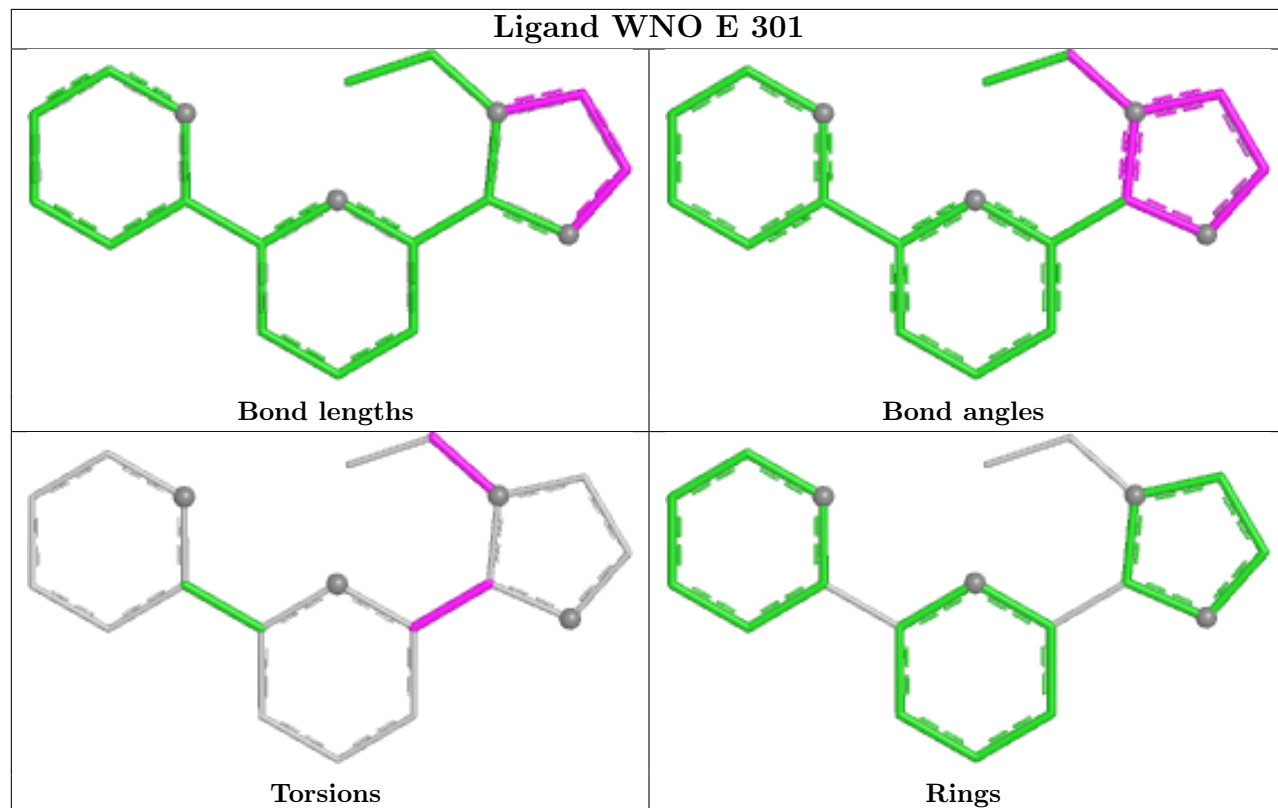
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

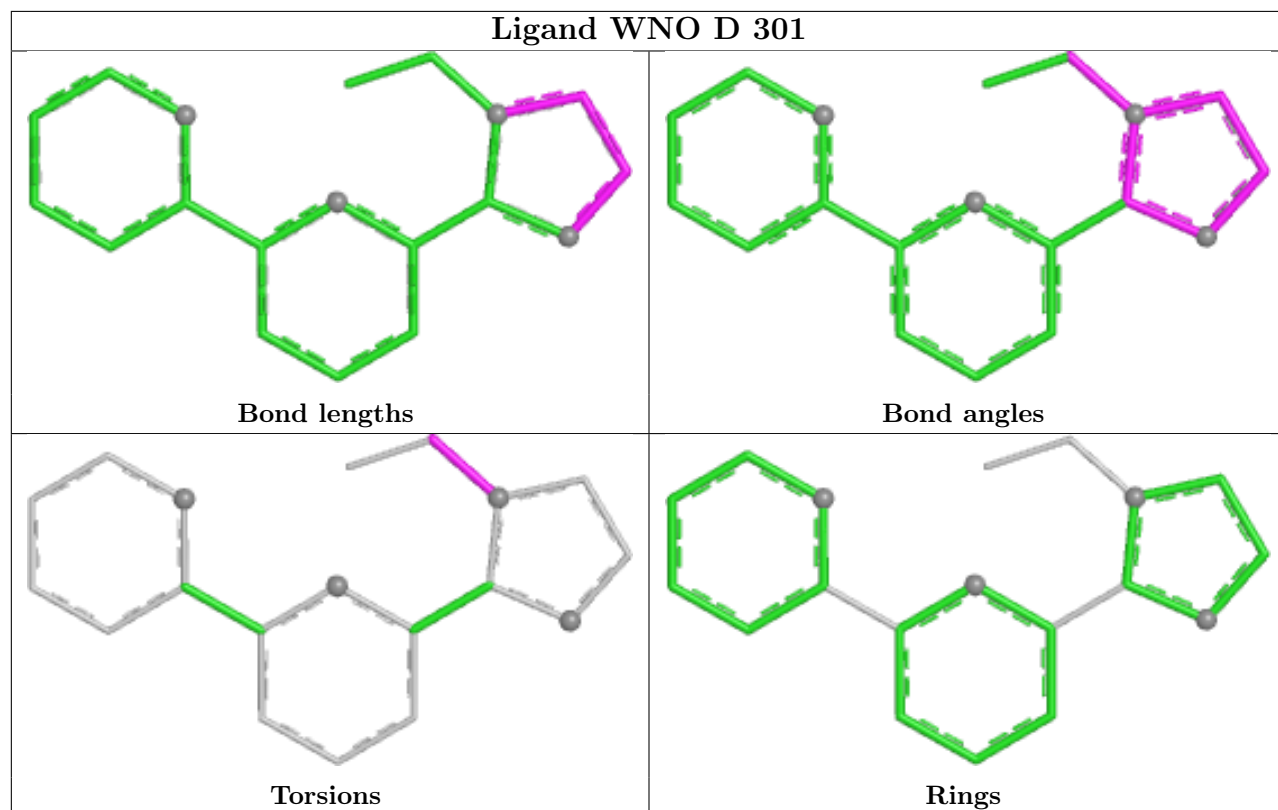
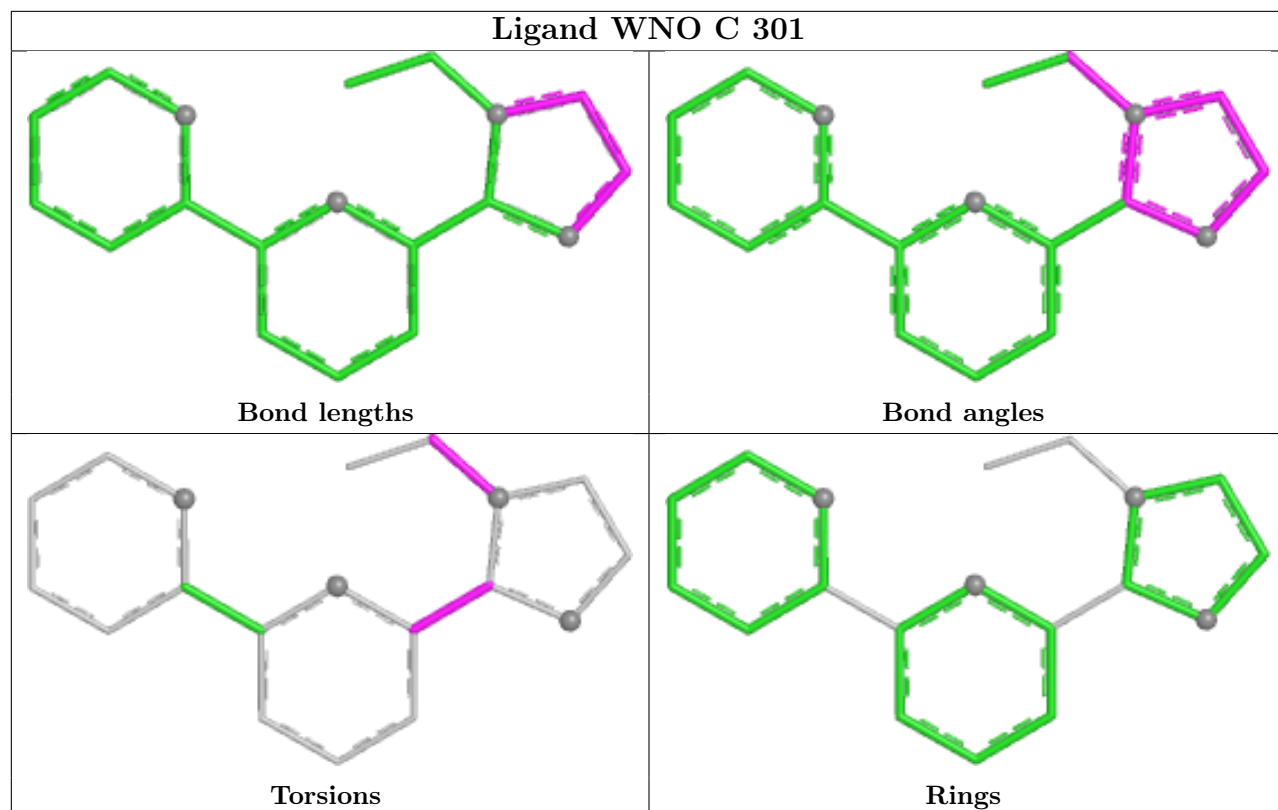


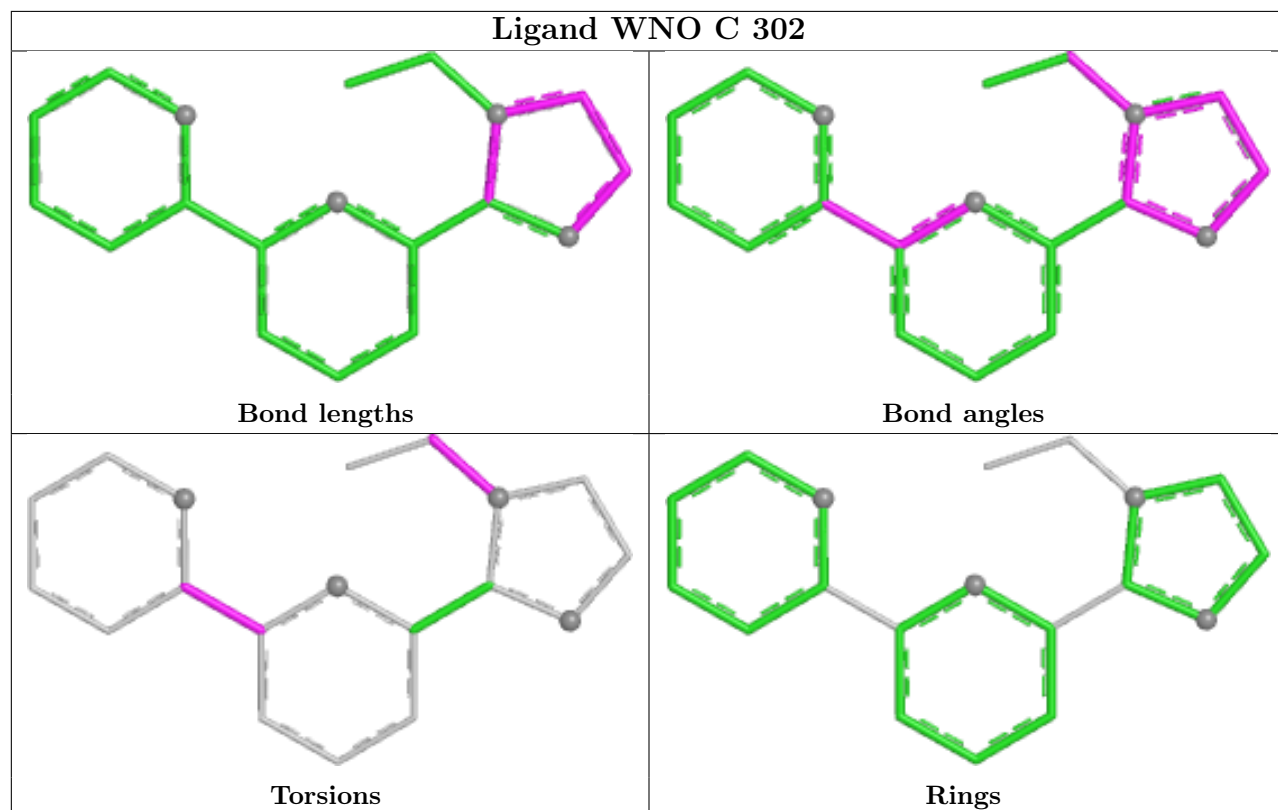
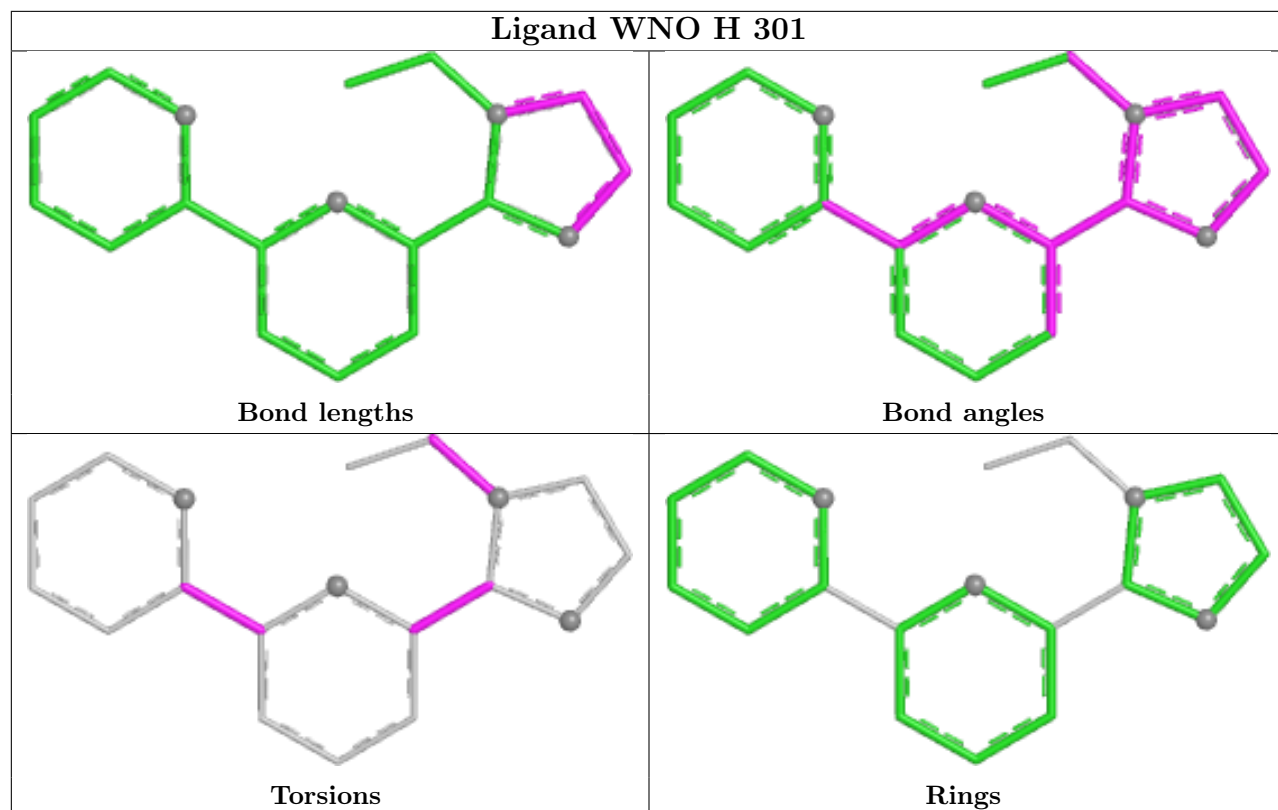
Ligand WNO G 301

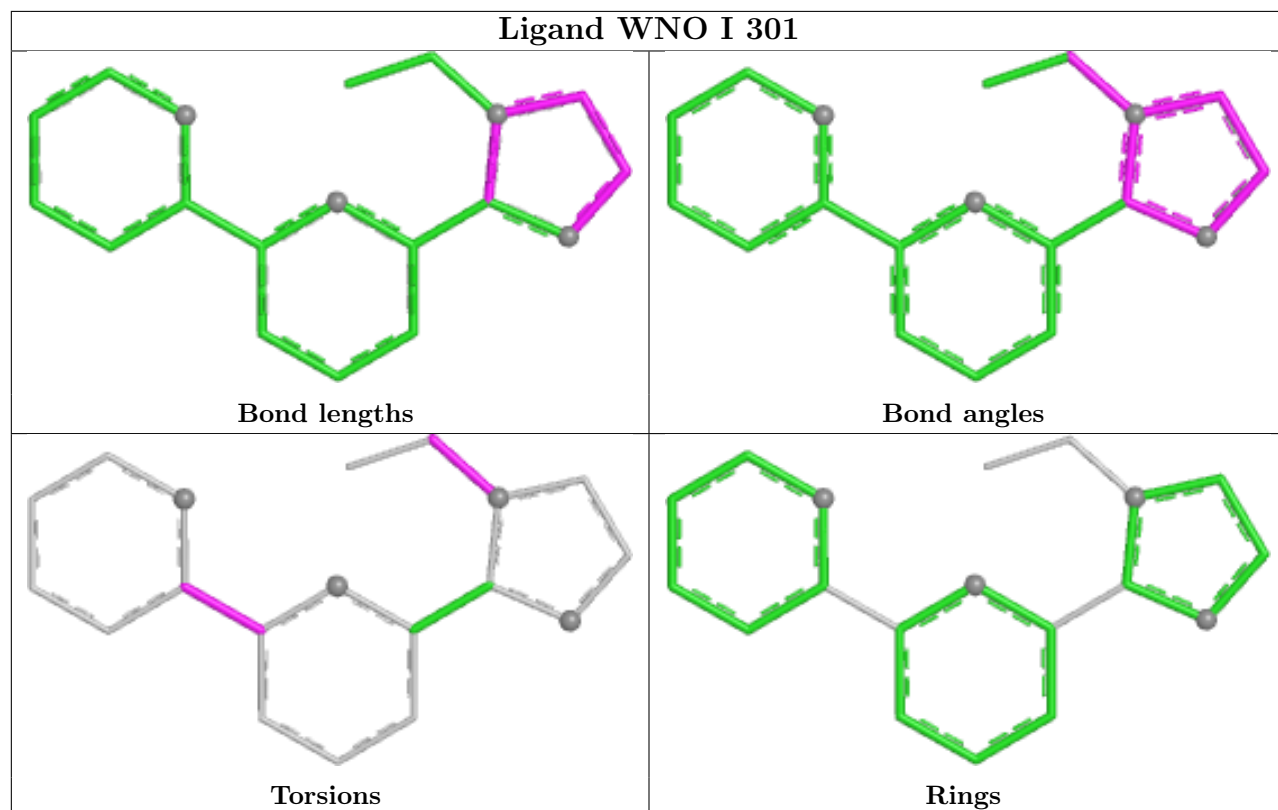
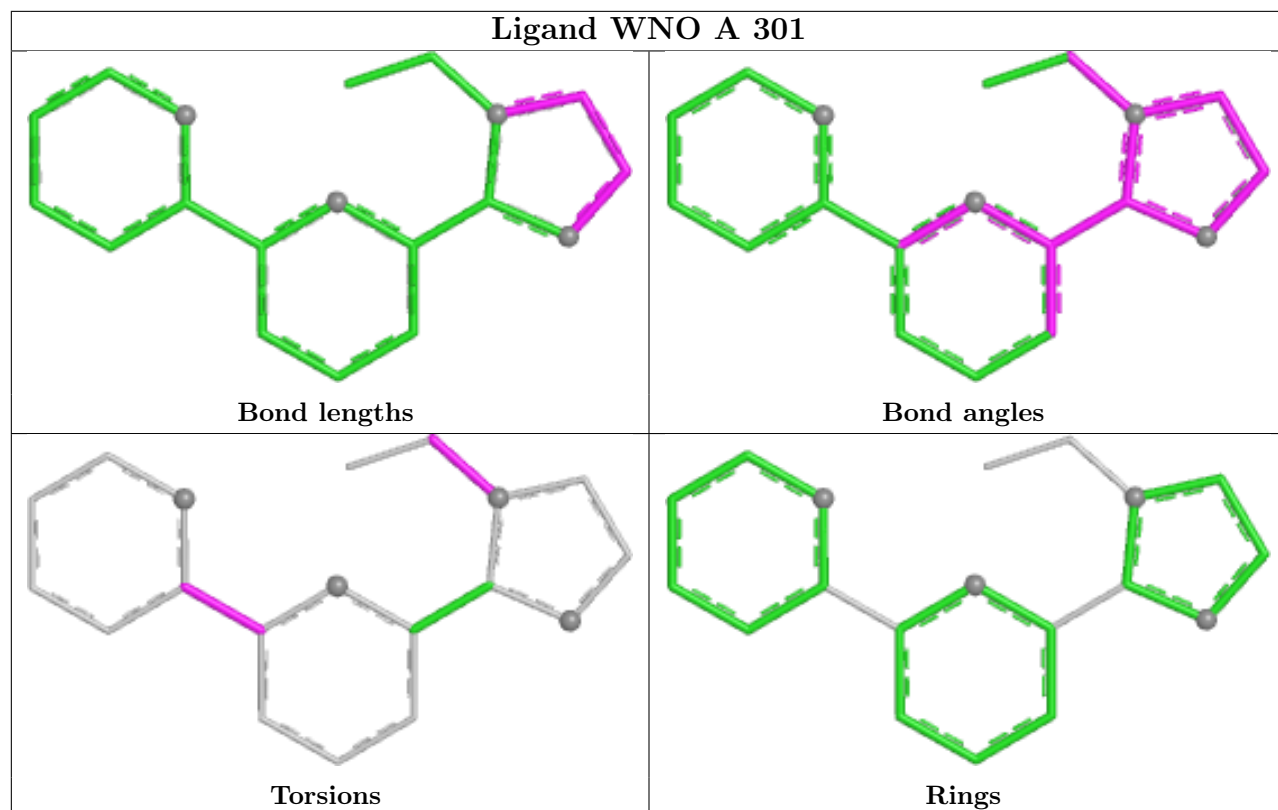


Ligand WNO E 301









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, 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	200/206 (97%)	0.20	2 (1%) 79 77	28, 45, 67, 84	0
1	B	199/206 (96%)	0.17	2 (1%) 79 77	32, 47, 75, 104	0
1	C	201/206 (97%)	0.18	6 (2%) 52 49	31, 45, 74, 92	0
1	D	201/206 (97%)	0.21	4 (1%) 65 62	28, 46, 72, 117	0
1	E	200/206 (97%)	0.15	3 (1%) 72 69	30, 44, 75, 100	0
1	F	200/206 (97%)	0.29	4 (2%) 65 62	27, 46, 74, 106	0
1	G	198/206 (96%)	0.20	1 (0%) 87 85	33, 45, 71, 100	0
1	H	199/206 (96%)	0.17	2 (1%) 79 77	30, 44, 72, 92	0
1	I	201/206 (97%)	0.39	4 (1%) 65 62	34, 51, 83, 125	0
1	J	199/206 (96%)	0.11	1 (0%) 87 85	30, 43, 67, 93	0
All	All	1998/2060 (96%)	0.21	29 (1%) 72 69	27, 45, 74, 125	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	20	PHE	4.9
1	I	20	PHE	4.0
1	H	20	PHE	3.7
1	A	20	PHE	3.5
1	F	224	GLY	3.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

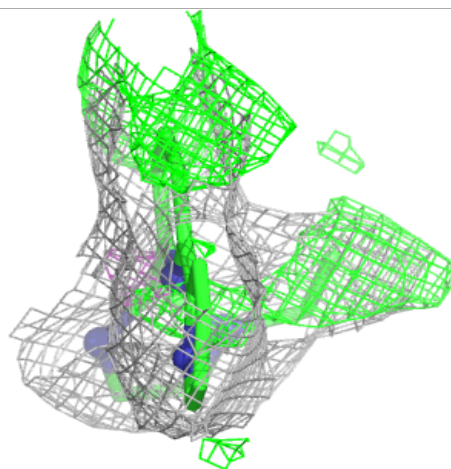
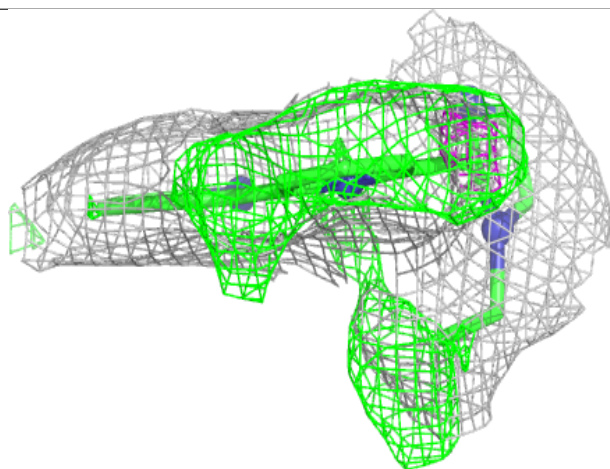
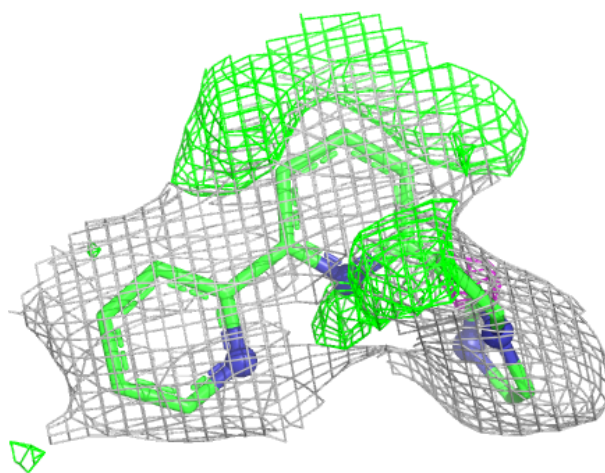
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	WNO	C	302	19/19	0.69	0.18	50,63,67,74	0
2	WNO	H	301	19/19	0.79	0.18	43,64,82,88	0
2	WNO	F	301	19/19	0.88	0.14	44,56,79,79	0
2	WNO	A	301	19/19	0.88	0.13	49,56,61,62	0
2	WNO	D	301	19/19	0.90	0.11	47,54,58,60	0
2	WNO	C	301	19/19	0.91	0.12	48,54,69,76	0
2	WNO	I	301	19/19	0.91	0.12	53,68,75,76	0
3	SO4	F	302	5/5	0.91	0.14	65,66,82,84	0
3	SO4	C	303	5/5	0.92	0.13	63,65,80,88	0
2	WNO	E	301	19/19	0.92	0.11	45,54,64,69	0
4	GOL	J	301	6/6	0.93	0.08	44,46,47,49	0
2	WNO	G	301	19/19	0.94	0.10	44,53,73,75	0
3	SO4	A	302	5/5	0.95	0.17	43,52,74,79	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.

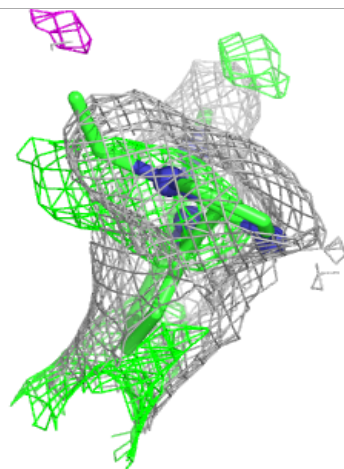
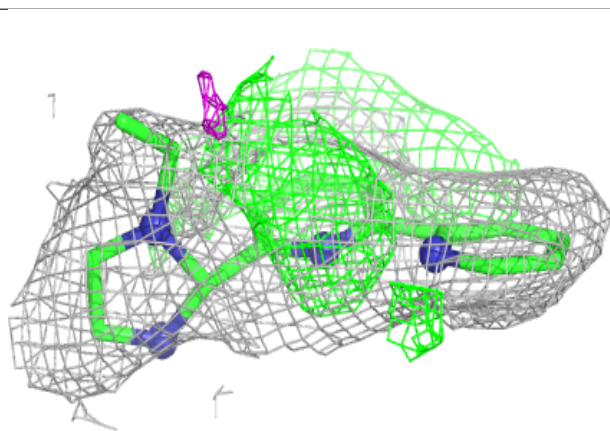
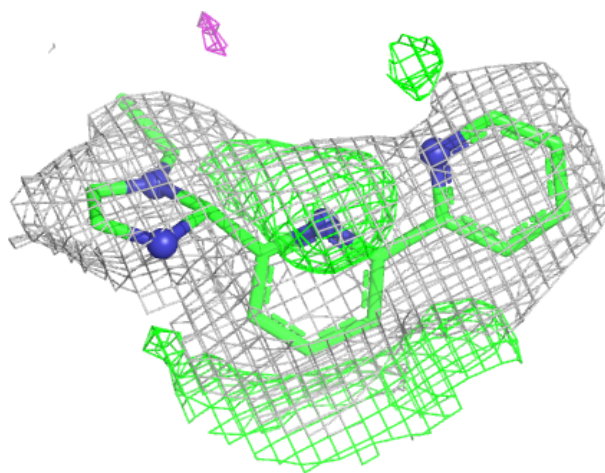
Electron density around WNO C 302:

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



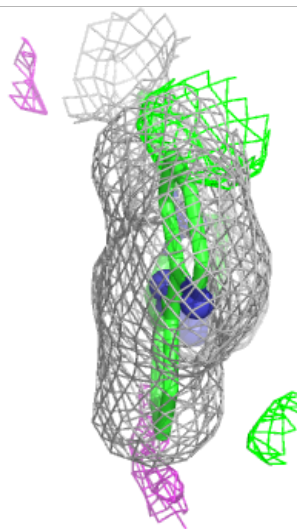
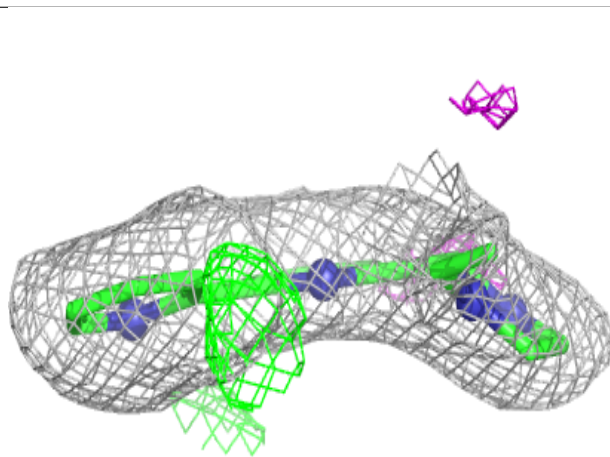
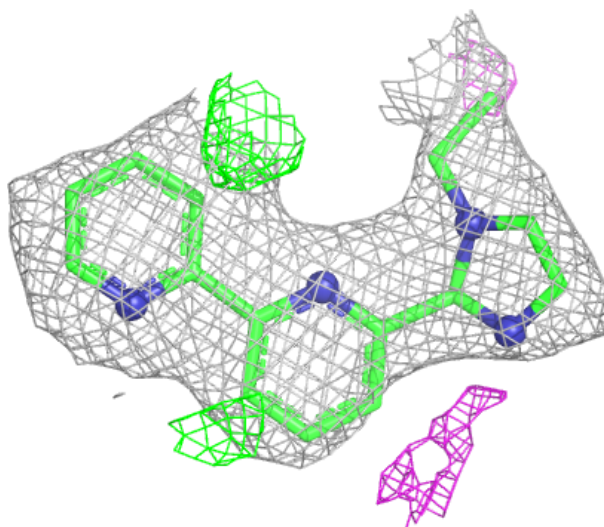
Electron density around WNO H 301:

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



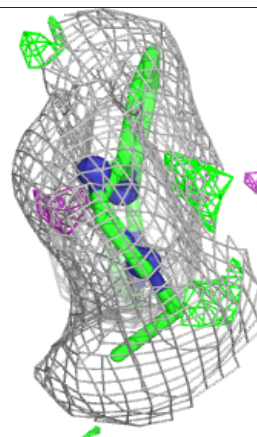
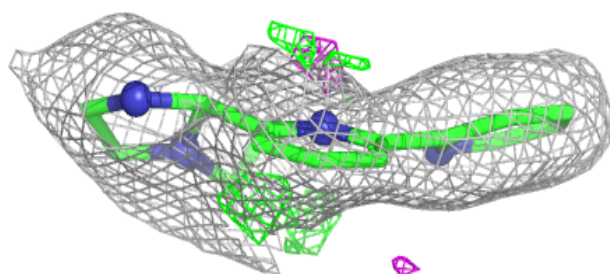
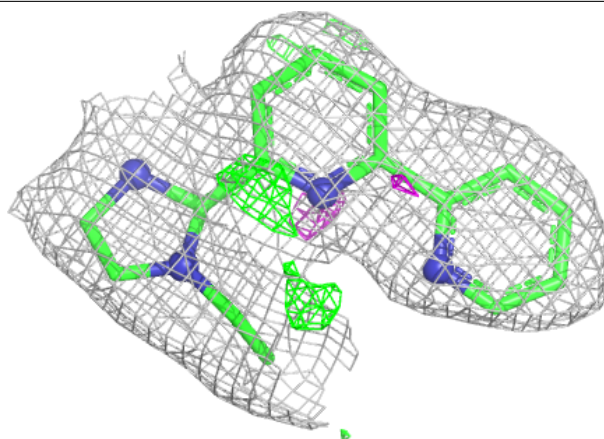
Electron density around WNO F 301:

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

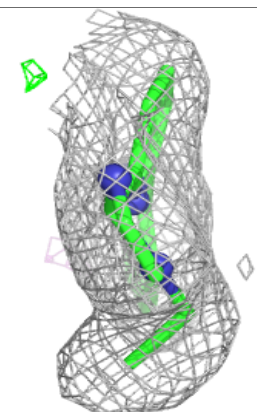
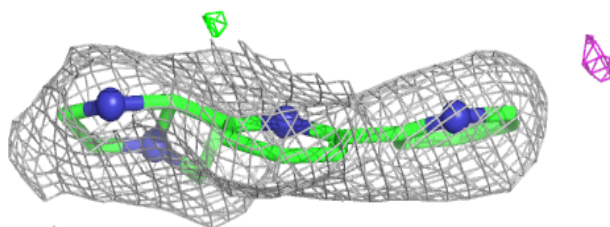
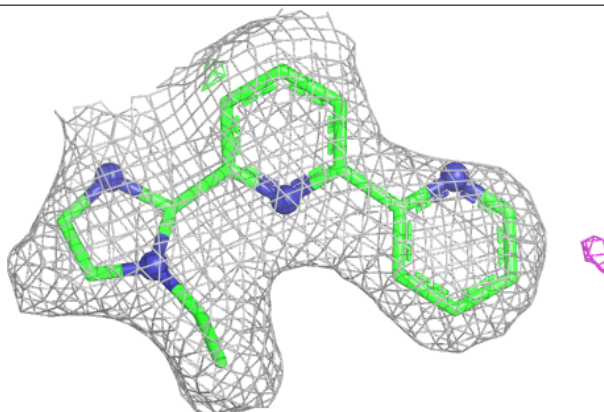


Electron density around WNO A 301:

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

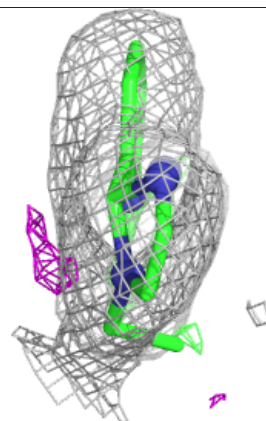
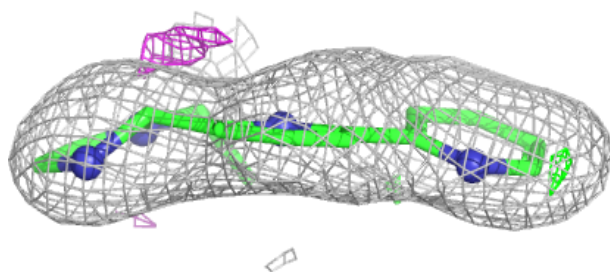
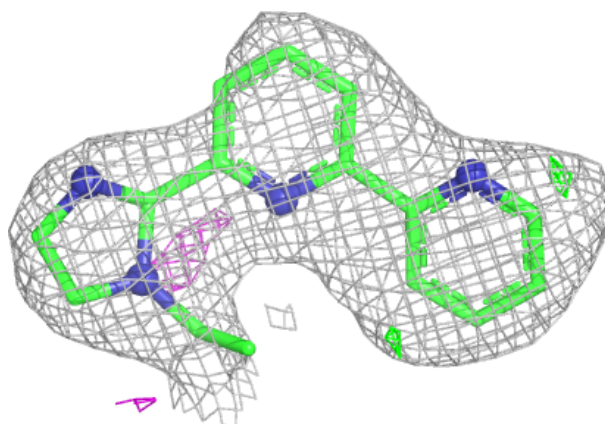
**Electron density around WNO D 301:**

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



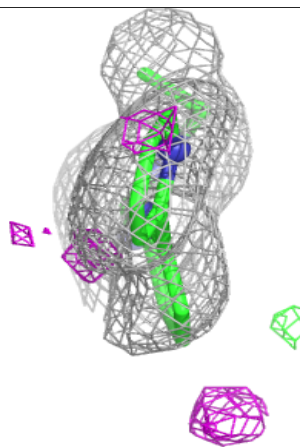
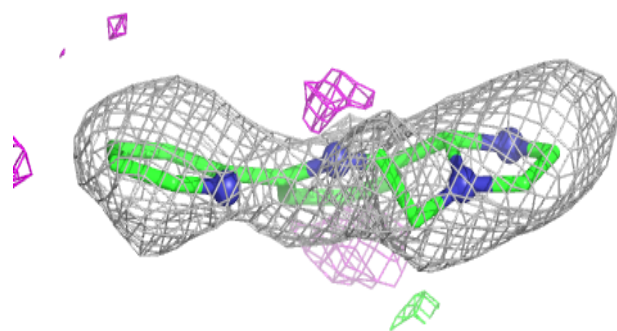
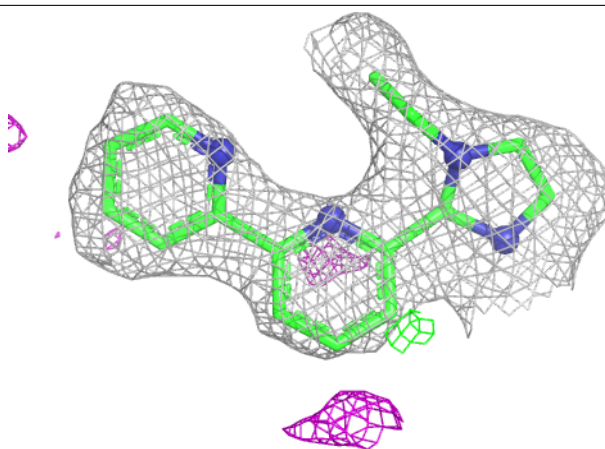
Electron density around WNO C 301:

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



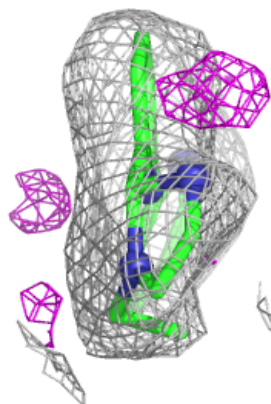
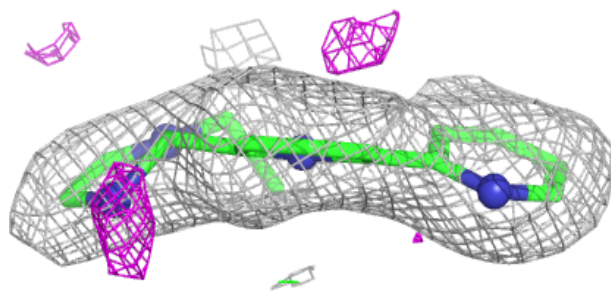
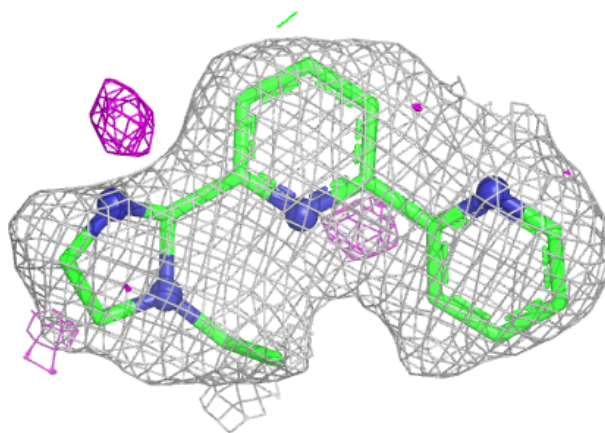
Electron density around WNO I 301:

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

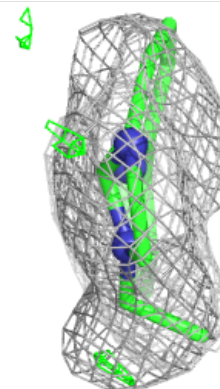
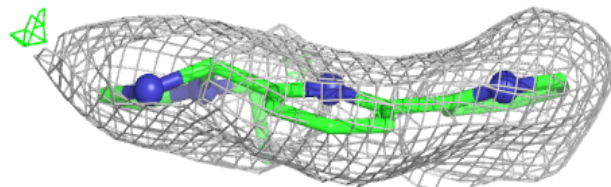
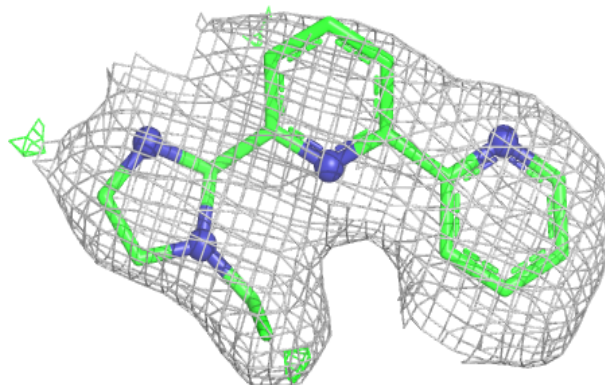


Electron density around WNO E 301:

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

**Electron density around WNO G 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.