



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2025 – 01:09 pm BST

PDB ID : 9QM8 / pdb\_00009qm8  
Title : X-ray structure of acetylcholine binding protein (AChBP) in complex with IOTA739  
Authors : Cederfelt, D.; Lund, B.A.; Boronat, P.; Hennig, S.; Dobritsch, D.; Danielson, U.H.  
Deposited on : 2025-03-22  
Resolution : 3.00 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](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.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

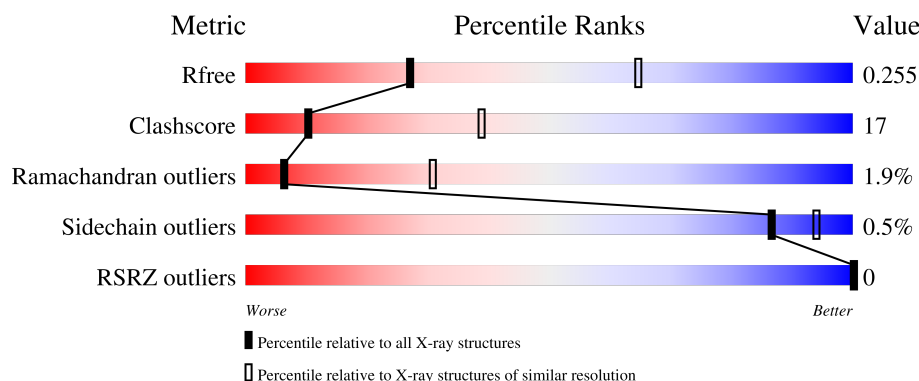
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.00 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))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	206	 66% 30% ..
1	B	206	 65% 32% ..
1	C	206	 68% 30% .
1	D	206	 67% 31% .

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Mol	Chain	Length	Quality of chain
1	E	206	 64% 34% .
1	F	206	 68% 28% ..
1	G	206	 58% 38% ..
1	H	206	 67% 31% .
1	I	206	 63% 34% .
1	J	206	 52% 42% ..

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
4	SO4	J	301	-	-	X	-

## 2 Entry composition

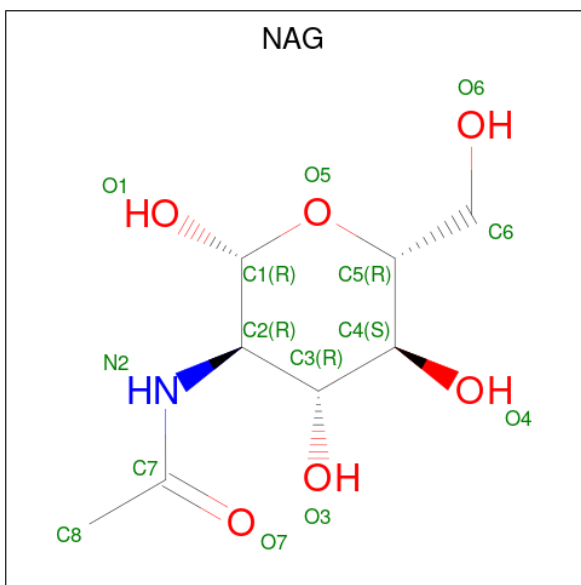
There are 5 unique types of molecules in this entry. The entry contains 16393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

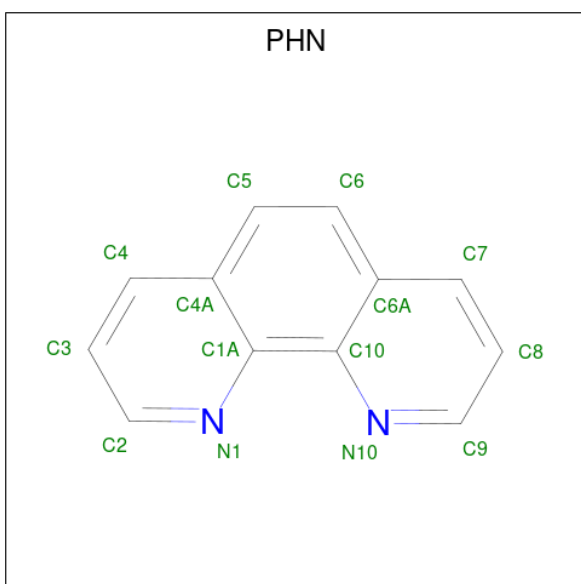
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1618	1014	277	322	5			
1	B	200	Total	C	N	O	S	0	0	0
			1602	1005	274	318	5			
1	C	201	Total	C	N	O	S	0	0	0
			1605	1007	275	318	5			
1	D	205	Total	C	N	O	S	0	0	0
			1638	1024	283	326	5			
1	E	203	Total	C	N	O	S	0	0	0
			1625	1017	278	325	5			
1	F	202	Total	C	N	O	S	0	0	0
			1614	1012	277	320	5			
1	G	200	Total	C	N	O	S	0	0	0
			1602	1005	274	318	5			
1	H	202	Total	C	N	O	S	0	0	0
			1614	1012	276	321	5			
1	I	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			
1	J	199	Total	C	N	O	S	0	0	0
			1594	1001	273	315	5			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



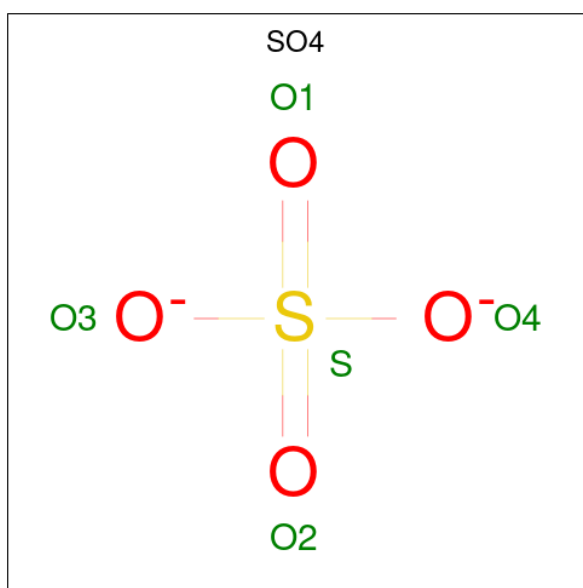
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1,10-PHENANTHROLINE (CCD ID: PHN) (formula:  $C_{12}H_8N_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	12	2		
3	B	1	Total	C	N	0	0
			14	12	2		
3	F	1	Total	C	N	0	0
			14	12	2		
3	G	1	Total	C	N	0	0
			14	12	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	14	Total	O	0	0
			14	14		
5	C	28	Total	O	0	0
			28	28		
5	D	19	Total	O	0	0
			19	19		

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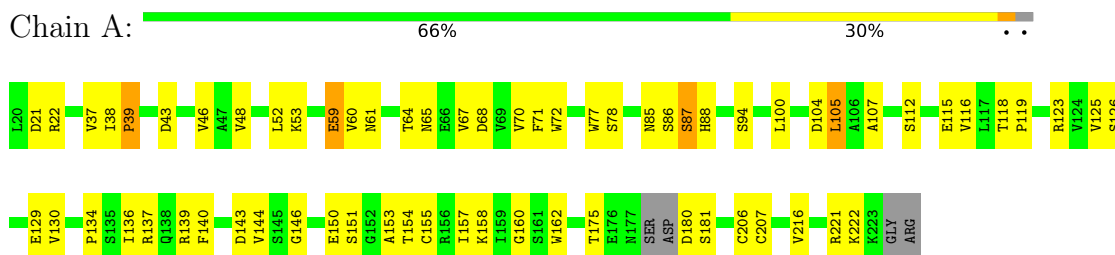
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	21	Total 21	O 21	0	0
5	F	13	Total 13	O 13	0	0
5	G	13	Total 13	O 13	0	0
5	H	23	Total 23	O 23	0	0
5	I	18	Total 18	O 18	0	0
5	J	12	Total 12	O 12	0	0

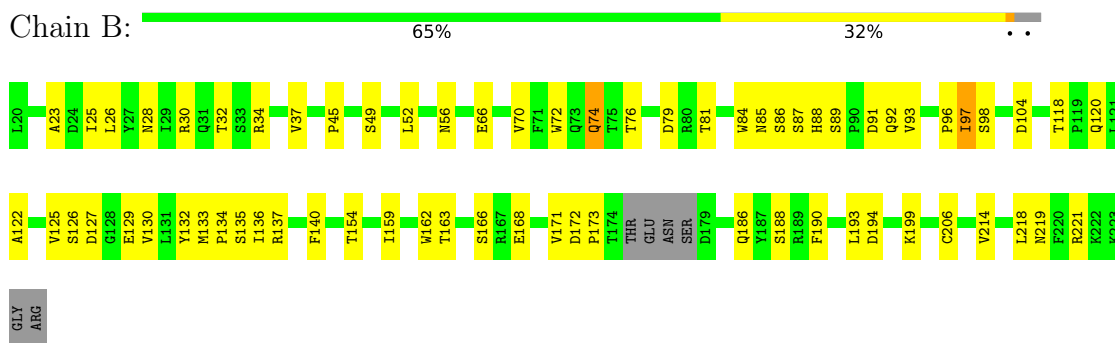
### 3 Residue-property plots

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.

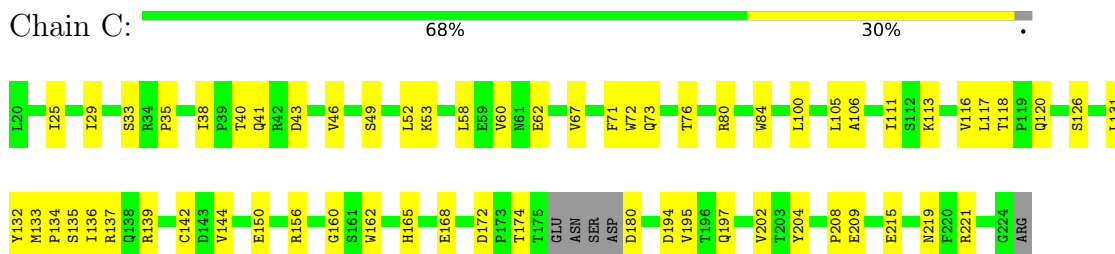
#### • Molecule 1: Acetylcholine-binding protein



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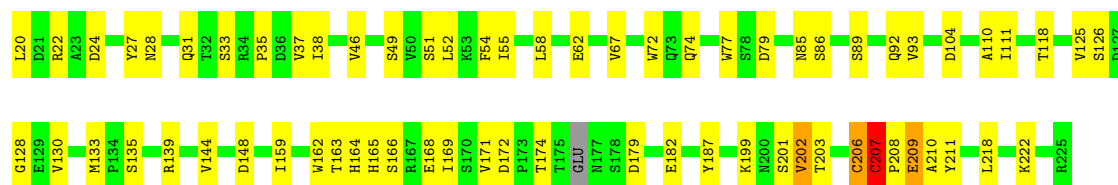


#### • Molecule 1: Acetylcholine-binding protein



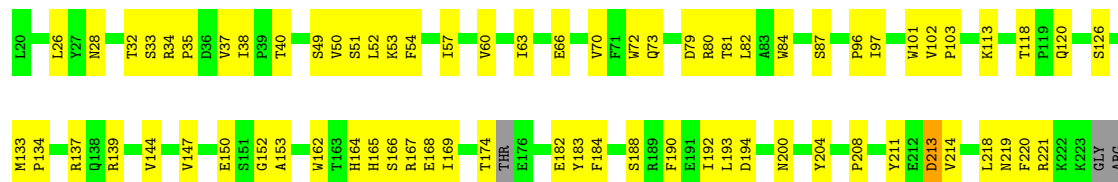
#### • Molecule 1: Acetylcholine-binding protein





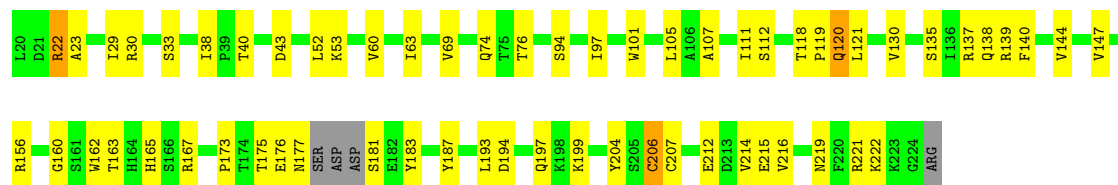
• Molecule 1: Acetylcholine-binding protein

Chain E: 64% 34%



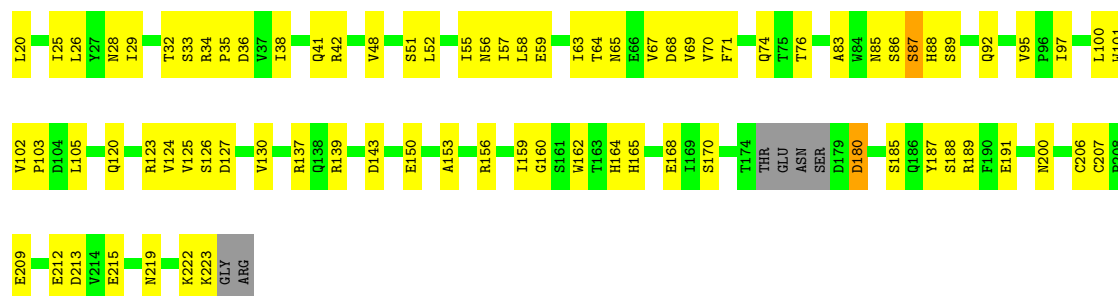
• Molecule 1: Acetylcholine-binding protein

Chain F: 68% 28%



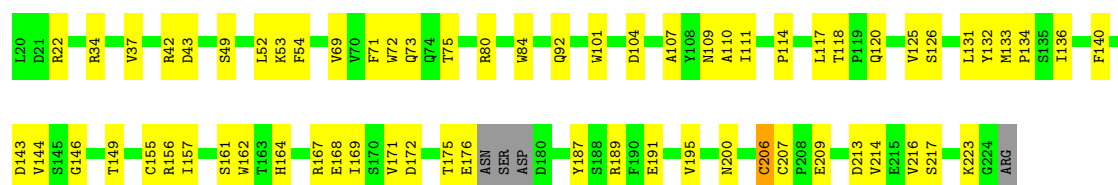
• Molecule 1: Acetylcholine-binding protein

Chain G: 58% 38%



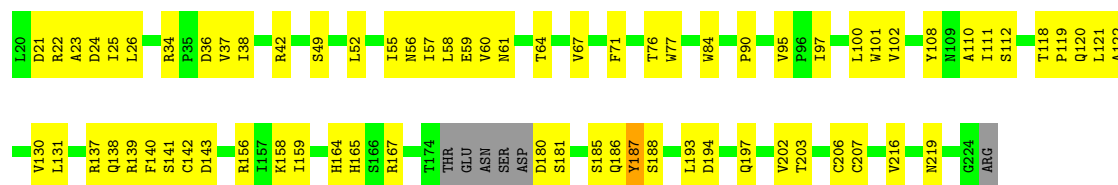
• Molecule 1: Acetylcholine-binding protein

Chain H: 67% 31%



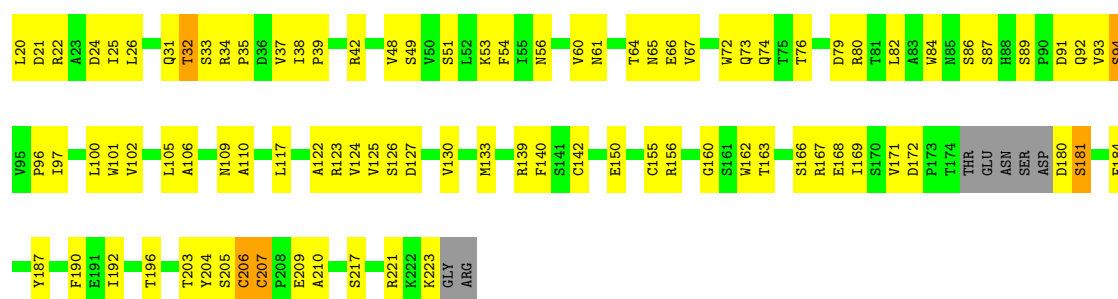
- Molecule 1: Acetylcholine-binding protein

Chain I:  63% 34%



- Molecule 1: Acetylcholine-binding protein

Chain J:  52% 42%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.95Å 117.85Å 239.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 3.00 49.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.59-3.00) 99.9 (49.59-3.00)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.01Å)	Xtriage
Refinement program	REFMAC 1.20.1 _4487, PHENIX 1.20.1 _4487	Depositor
R, $R_{free}$	0.224 , 0.253 0.237 , 0.255	Depositor DCC
$R_{free}$ test set	41407 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	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 28.69 % 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 1.7621e-03. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, PHN

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	0.50	0/1653	0.78	0/2255
1	B	0.55	0/1637	0.77	0/2233
1	C	0.56	0/1640	0.77	0/2237
1	D	0.51	0/1673	0.82	0/2281
1	E	0.58	1/1660 (0.1%)	0.83	0/2264
1	F	0.49	0/1649	0.77	0/2249
1	G	0.52	0/1637	0.82	0/2233
1	H	0.49	0/1649	0.75	0/2249
1	I	0.51	0/1633	0.76	0/2227
1	J	0.48	0/1629	0.71	0/2222
All	All	0.52	1/16460 (0.0%)	0.78	0/22450

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	A	0	1
1	B	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81	THR	CA-C	6.38	1.61	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	B	206	CYS	Peptide
1	E	213	ASP	Peptide
1	F	206	CYS	Peptide
1	F	22	ARG	Sidechain

## 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	1618	0	1564	46	0
1	B	1602	0	1549	54	0
1	C	1605	0	1556	53	0
1	D	1638	0	1584	56	0
1	E	1625	0	1566	61	0
1	F	1614	0	1564	48	0
1	G	1602	0	1550	64	0
1	H	1614	0	1562	47	0
1	I	1598	0	1549	60	0
1	J	1594	0	1546	95	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
2	E	14	0	13	0	0
3	A	14	0	8	0	0
3	B	14	0	8	0	0
3	F	14	0	8	5	0
3	G	14	0	8	0	0
4	F	5	0	0	1	0
4	J	5	0	0	3	0
5	A	14	0	0	1	0
5	B	14	0	0	4	0
5	C	28	0	0	21	0
5	D	19	0	0	2	0
5	E	21	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	13	0	0	1	0
5	G	13	0	0	8	0
5	H	23	0	0	2	0
5	I	18	0	0	6	0
5	J	12	0	0	9	0
All	All	16393	0	15661	535	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 17.

The worst 5 of 535 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:175:THR:HG22	1:F:176:GLU:H	1.08	1.10
1:F:199:LYS:NZ	1:F:212:GLU:OE1	1.93	1.01
1:C:135:SER:HA	5:C:303:HOH:O	1.58	0.99
1:D:206:CYS:SG	1:D:207:CYS:N	2.40	0.94
1:C:142:CYS:SG	5:C:328:HOH:O	2.26	0.93

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	198/206 (96%)	164 (83%)	25 (13%)	9 (4%)	2	12
1	B	196/206 (95%)	163 (83%)	30 (15%)	3 (2%)	8	36
1	C	197/206 (96%)	170 (86%)	24 (12%)	3 (2%)	8	36
1	D	201/206 (98%)	170 (85%)	26 (13%)	5 (2%)	4	24
1	E	199/206 (97%)	175 (88%)	21 (11%)	3 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	198/206 (96%)	182 (92%)	13 (7%)	3 (2%)	8	36
1	G	196/206 (95%)	176 (90%)	18 (9%)	2 (1%)	13	46
1	H	198/206 (96%)	178 (90%)	18 (9%)	2 (1%)	13	46
1	I	196/206 (95%)	165 (84%)	29 (15%)	2 (1%)	13	46
1	J	195/206 (95%)	166 (85%)	23 (12%)	6 (3%)	3	19
All	All	1974/2060 (96%)	1709 (87%)	227 (12%)	38 (2%)	6	31

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	87	SER
1	E	87	SER
1	F	43	ASP
1	G	87	SER

### 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	189/192 (98%)	188 (100%)	1 (0%)	86	94
1	B	187/192 (97%)	187 (100%)	0	100	100
1	C	187/192 (97%)	187 (100%)	0	100	100
1	D	191/192 (100%)	189 (99%)	2 (1%)	73	88
1	E	190/192 (99%)	190 (100%)	0	100	100
1	F	188/192 (98%)	188 (100%)	0	100	100
1	G	187/192 (97%)	187 (100%)	0	100	100
1	H	188/192 (98%)	185 (98%)	3 (2%)	58	82
1	I	186/192 (97%)	186 (100%)	0	100	100
1	J	186/192 (97%)	183 (98%)	3 (2%)	58	82
All	All	1879/1920 (98%)	1870 (100%)	9 (0%)	86	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	206	CYS
1	J	207	CYS
1	H	155	CYS
1	H	206	CYS
1	H	207	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	56	ASN
1	J	73	GLN
1	I	61	ASN
1	I	200	ASN
1	D	186	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	NAG	B	301	1	14,14,15	1.42	3 (21%)	17,19,21	0.79	0
3	PHN	F	301	-	16,16,16	0.81	0	22,22,22	0.78	0
2	NAG	E	301	1	14,14,15	1.07	2 (14%)	17,19,21	1.07	1 (5%)
4	SO4	J	301	-	4,4,4	0.12	0	6,6,6	0.24	0
3	PHN	A	302	-	16,16,16	0.69	0	22,22,22	0.65	0
3	PHN	B	302	-	16,16,16	0.82	0	22,22,22	0.63	0
2	NAG	A	301	1	14,14,15	2.00	2 (14%)	17,19,21	1.47	1 (5%)
4	SO4	F	302	-	4,4,4	0.17	0	6,6,6	0.23	0
3	PHN	G	301	-	16,16,16	0.73	0	22,22,22	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	301	1	-	2/6/23/26	0/1/1/1
3	PHN	F	301	-	-	-	0/3/3/3
2	NAG	E	301	1	-	1/6/23/26	0/1/1/1
3	PHN	A	302	-	-	-	0/3/3/3
3	PHN	B	302	-	-	-	0/3/3/3
2	NAG	A	301	1	-	2/6/23/26	0/1/1/1
3	PHN	G	301	-	-	-	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAG	O5-C1	6.97	1.54	1.43
2	B	301	NAG	O5-C1	-3.85	1.37	1.43
2	B	301	NAG	C1-C2	2.86	1.56	1.52
2	E	301	NAG	C1-C2	2.59	1.56	1.52
2	E	301	NAG	O5-C1	2.28	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAG	C1-O5-C5	5.39	119.49	112.19
2	E	301	NAG	O3-C3-C2	2.82	115.31	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAG	C8-C7-N2-C2
2	B	301	NAG	O7-C7-N2-C2
2	A	301	NAG	C4-C5-C6-O6
2	E	301	NAG	O5-C5-C6-O6
2	A	301	NAG	O5-C5-C6-O6

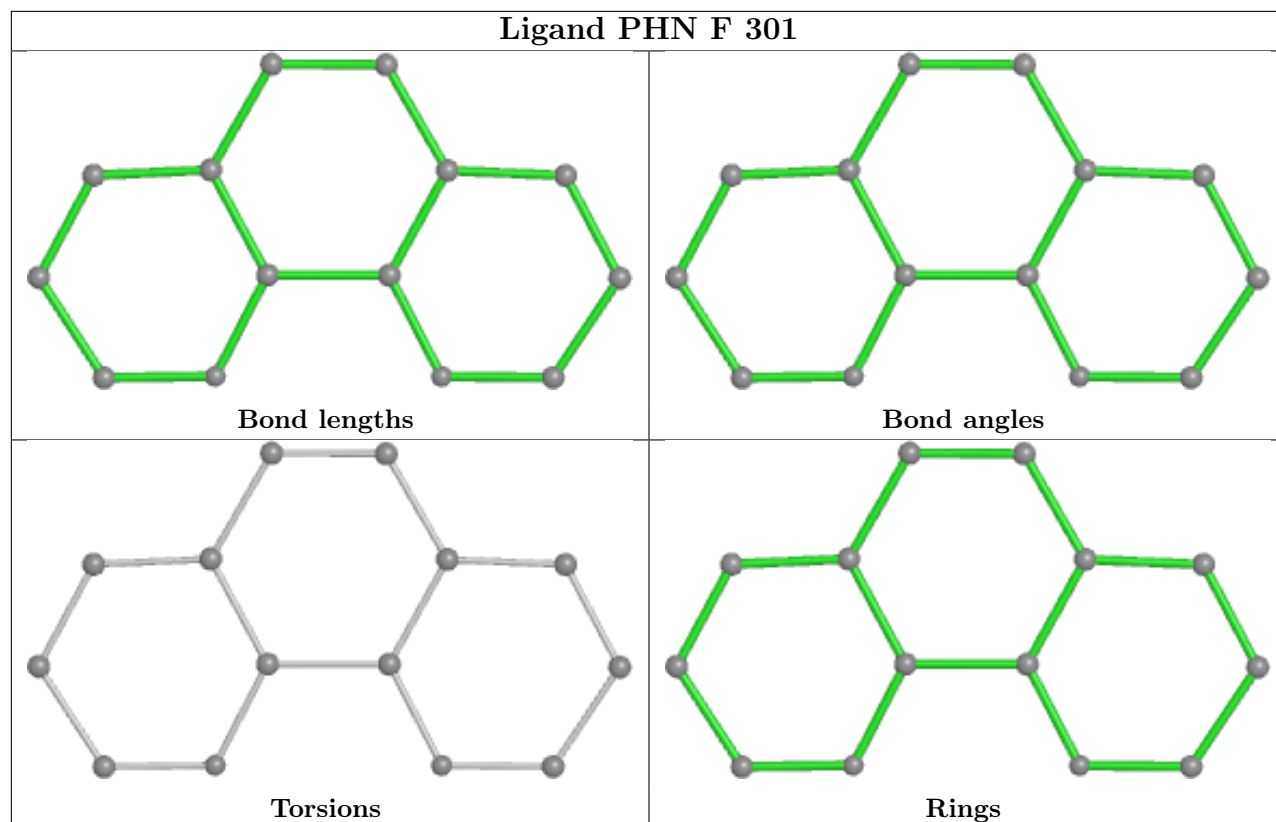
There are no ring outliers.

5 monomers are involved in 11 short contacts:

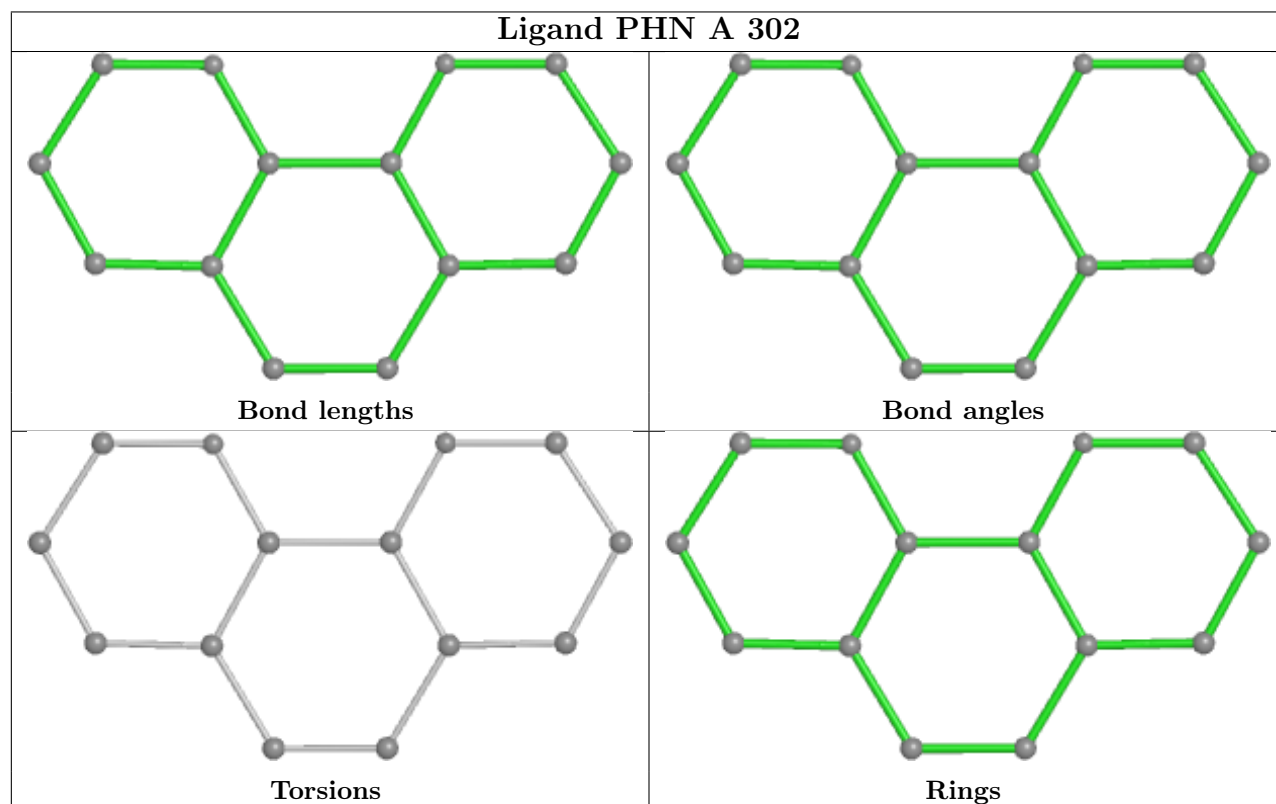
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAG	1	0
3	F	301	PHN	5	0
4	J	301	SO4	3	0
2	A	301	NAG	1	0
4	F	302	SO4	1	0

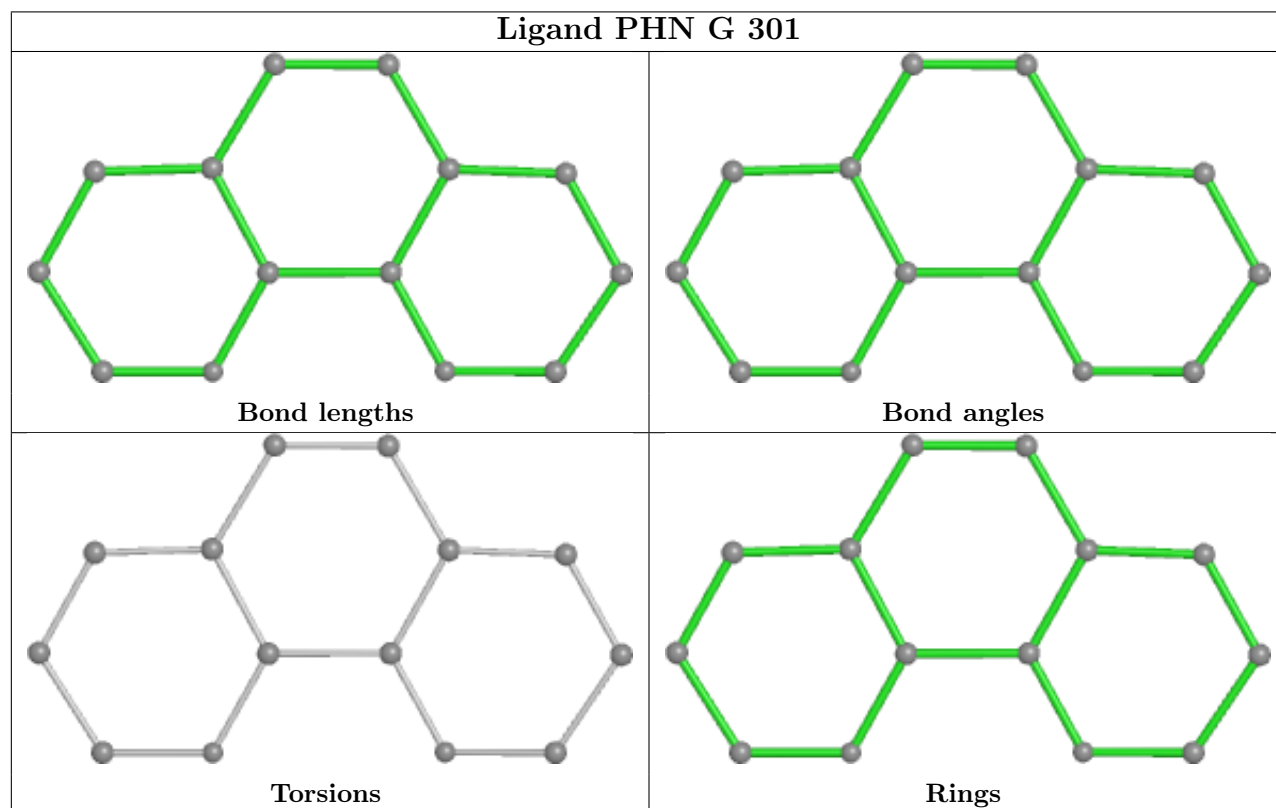
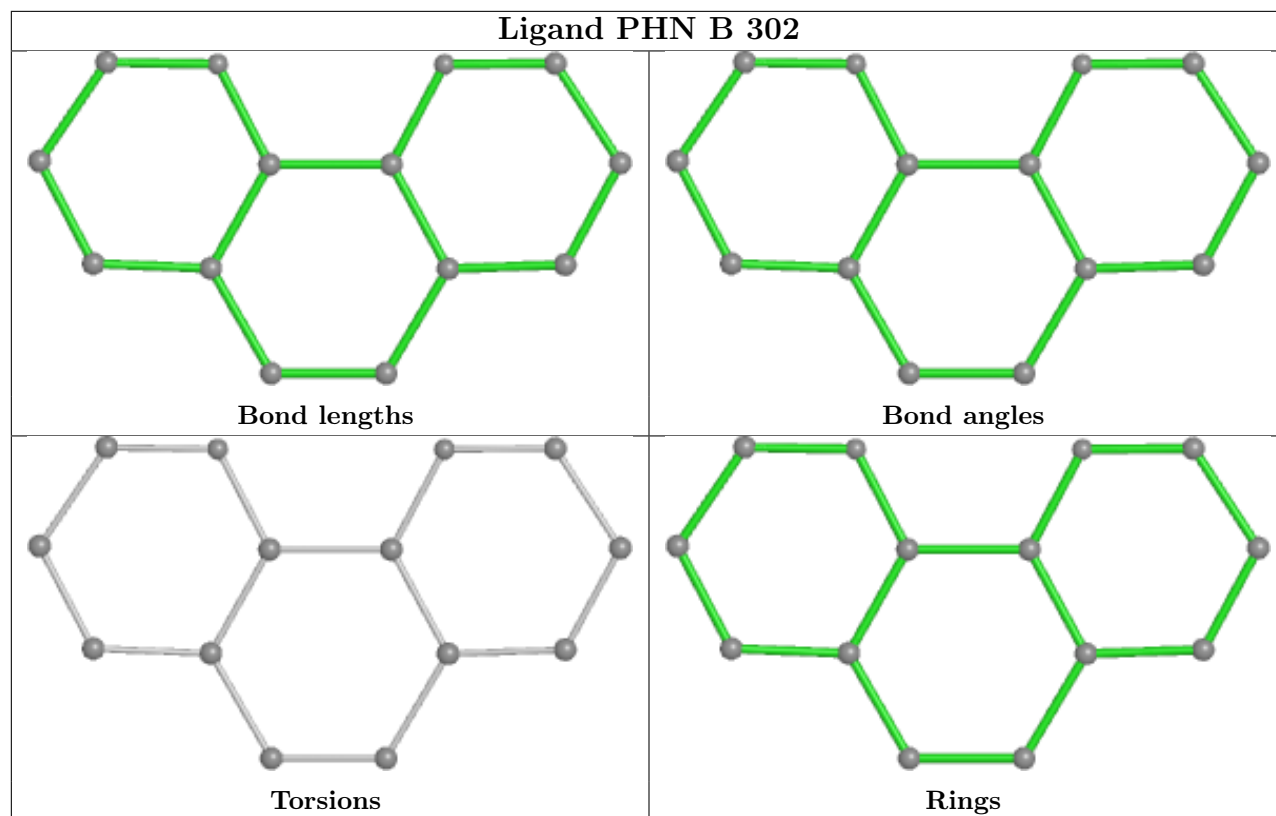
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand PHN F 301



## Ligand PHN A 302





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	202/206 (98%)	-0.84	0 100 100	47, 82, 120, 167	0
1	B	200/206 (97%)	-0.79	0 100 100	52, 85, 120, 164	0
1	C	201/206 (97%)	-0.80	0 100 100	58, 86, 128, 178	0
1	D	205/206 (99%)	-0.75	0 100 100	55, 85, 125, 206	0
1	E	203/206 (98%)	-0.77	0 100 100	57, 80, 124, 146	0
1	F	202/206 (98%)	-0.80	0 100 100	53, 89, 129, 204	0
1	G	200/206 (97%)	-0.78	0 100 100	55, 85, 127, 150	0
1	H	202/206 (98%)	-0.76	0 100 100	60, 88, 142, 215	0
1	I	200/206 (97%)	-0.64	0 100 100	59, 94, 148, 197	0
1	J	199/206 (96%)	-0.65	0 100 100	59, 96, 141, 253	0
All	All	2014/2060 (97%)	-0.76	0 100 100	47, 87, 133, 253	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

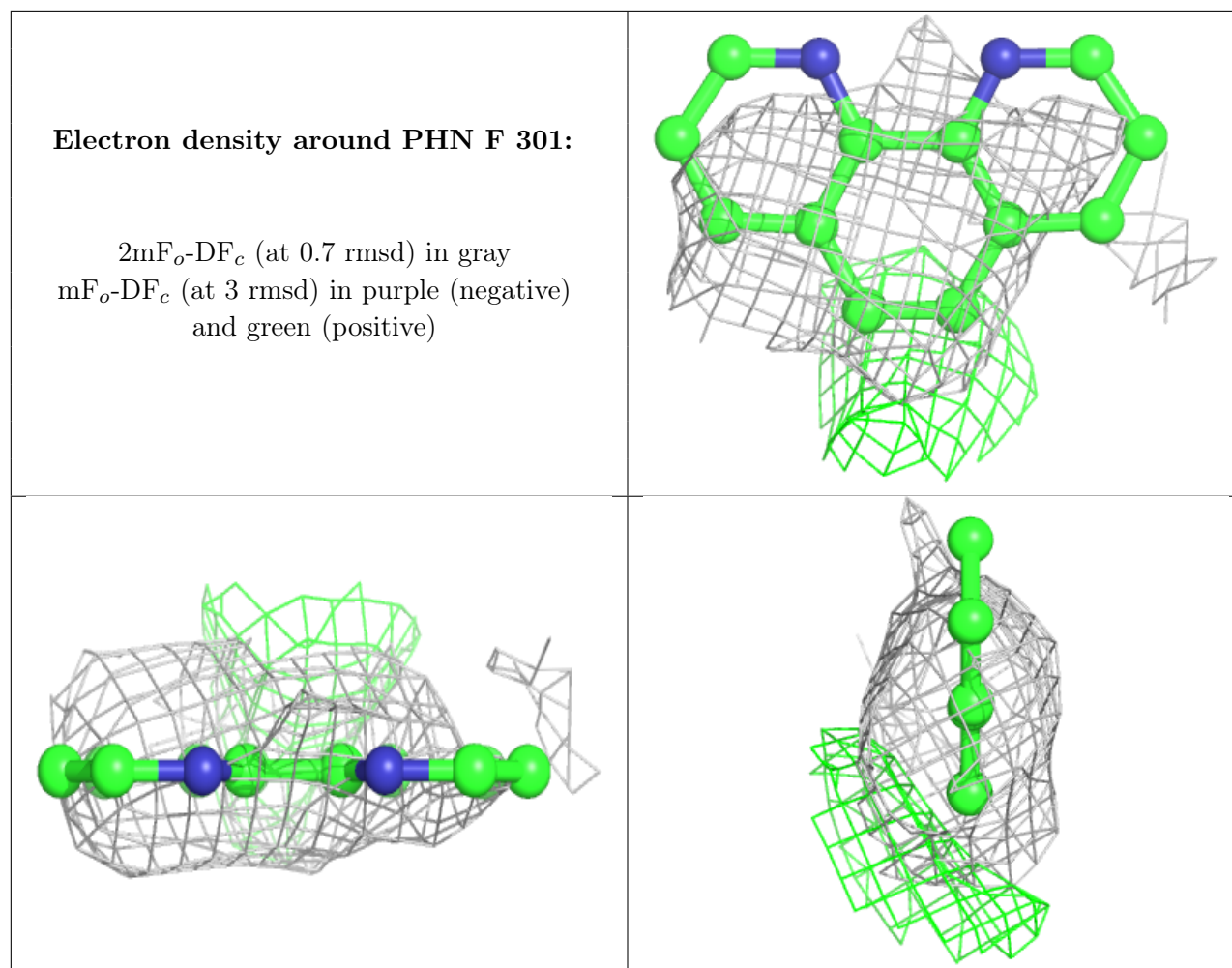
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

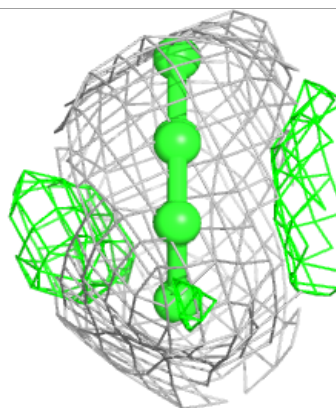
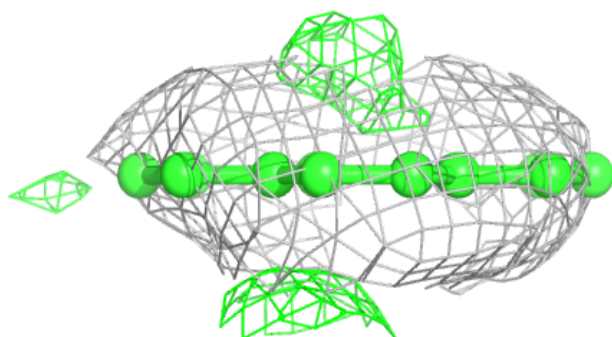
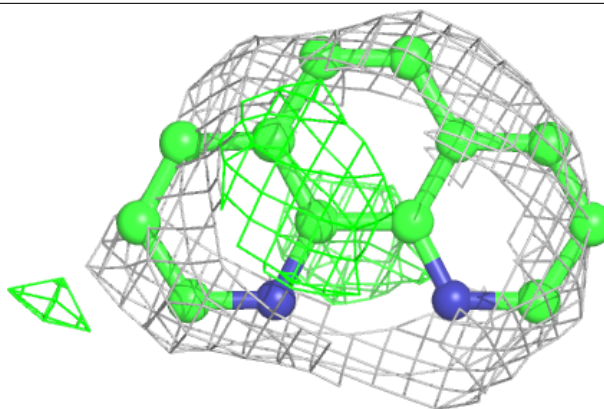
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	E	301	14/15	0.54	0.13	98,151,169,171	0
2	NAG	B	301	14/15	0.59	0.09	105,143,186,191	0
2	NAG	A	301	14/15	0.64	0.08	116,148,173,182	0
3	PHN	F	301	14/14	0.78	0.17	112,140,168,180	0
4	SO4	J	301	5/5	0.88	0.09	269,295,301,327	0
3	PHN	B	302	14/14	0.91	0.14	110,139,163,166	0
3	PHN	G	301	14/14	0.93	0.10	118,132,174,178	0
4	SO4	F	302	5/5	0.93	0.10	136,176,189,207	0
3	PHN	A	302	14/14	0.93	0.10	84,109,125,136	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.

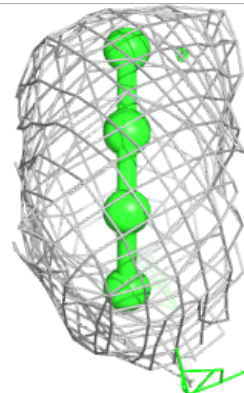
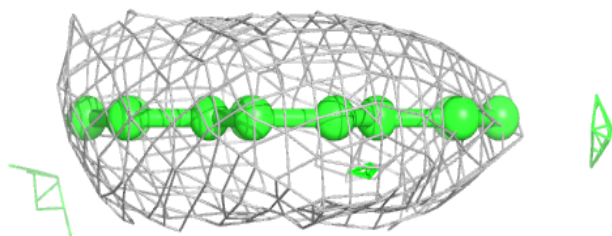
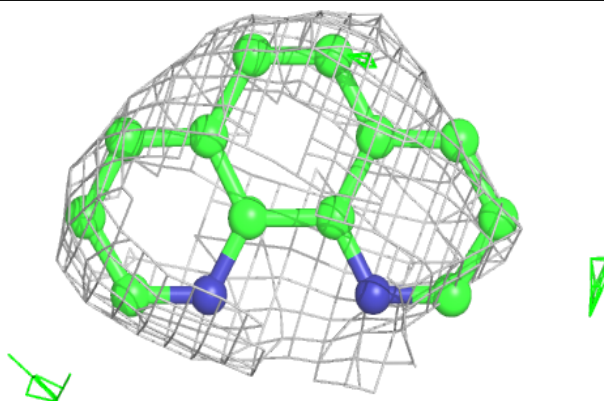


**Electron density around PHN B 302:**

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

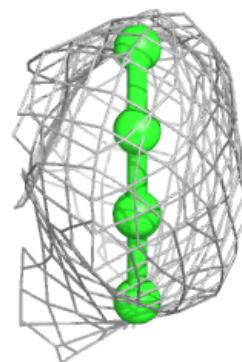
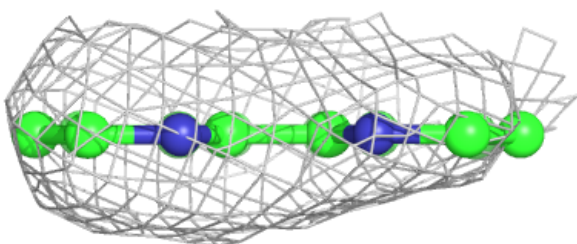
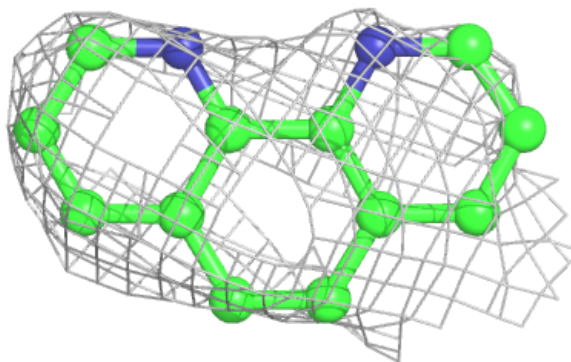
**Electron density around PHN G 301:**

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



**Electron density around PHN A 302:**

$2mF_o-DF_c$  (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.