



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 05:31 pm GMT

PDB ID : 6I96  
Title : Structure of the ferrioxamine B transporter FoxA from *Pseudomonas aeruginosa* in complex with ferrioxamine B  
Authors : Josts, I.; Tidow, H.  
Deposited on : 2018-11-22  
Resolution : 1.85 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)

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<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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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)	:	2.39

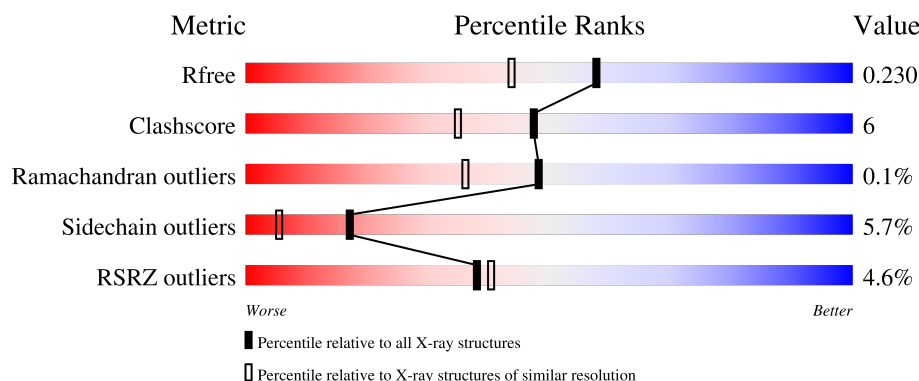
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	677	<div> <div>5%</div> <div>82%</div> <div>14%</div> <div>...</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0UE	A	901	X	-	-	-

## 2 Entry composition [i](#)

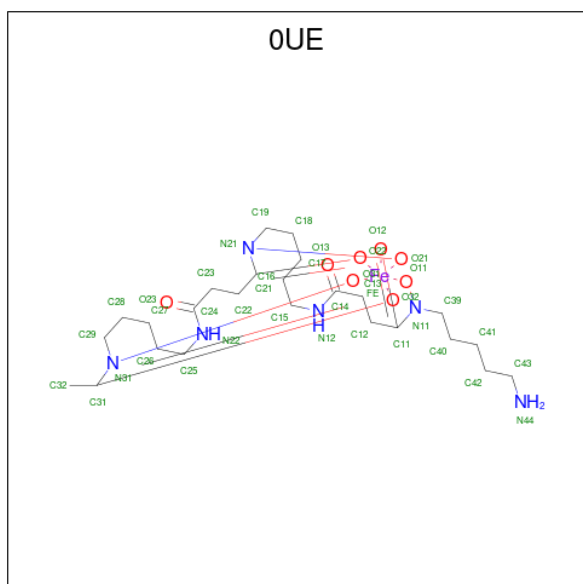
There are 7 unique types of molecules in this entry. The entry contains 5945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferric hydroxamate uptake.

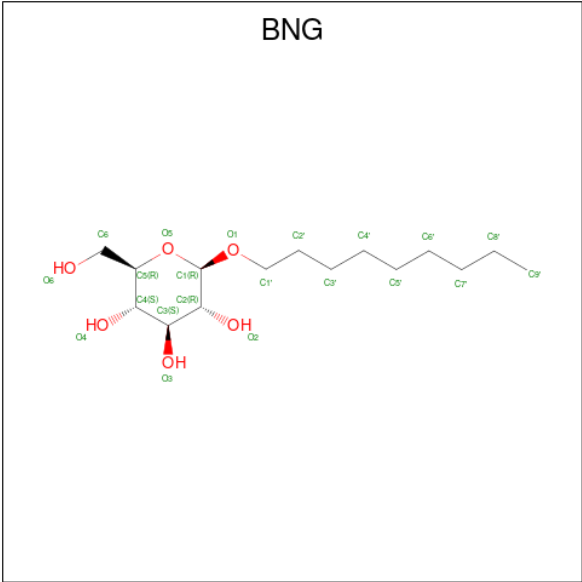
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	677	5325	3345	910	1059	11	0	0	0

- Molecule 2 is Ferrioxamine B (three-letter code: 0UE) (formula:  $C_{25}H_{45}FeN_6O_8$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	40	25	1	6	8	0	0

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula:  $C_{15}H_{30}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		
3	A	1	Total	C	O	0	0
			21	15	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		

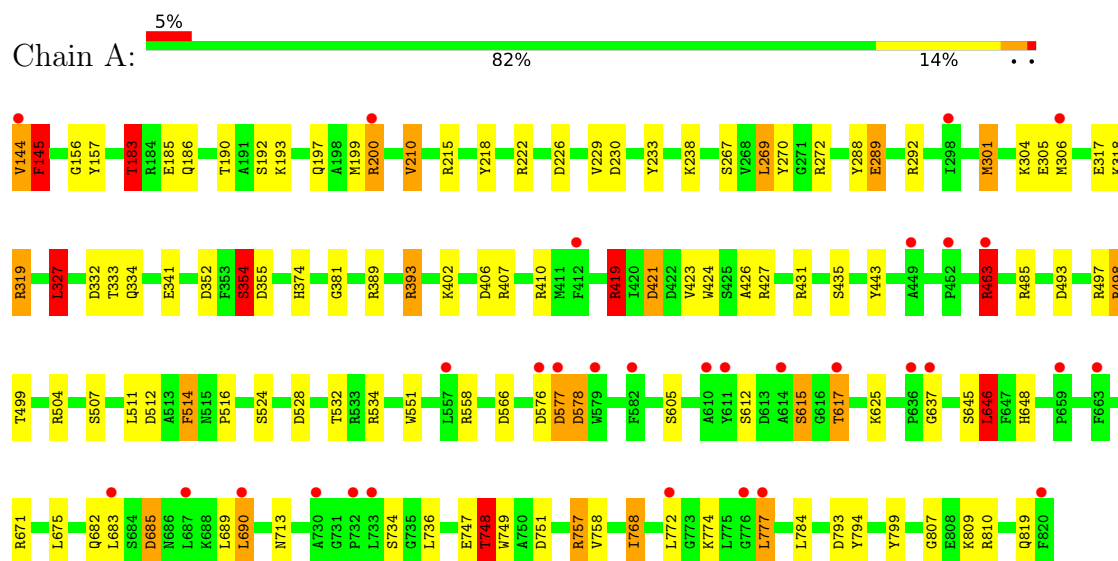
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	257	Total	O	0	0
			257	257		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ferric hydroxamate uptake



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.89Å 94.89Å 177.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.18 – 1.85 82.18 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (82.18-1.85) 99.2 (82.18-1.85)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.181 , 0.219 0.191 , 0.230	Depositor DCC
$R_{free}$ test set	3991 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OUE, SO4, BNG, NA

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	1.36	21/5451 (0.4%)	1.34	57/7397 (0.8%)

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	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	ASP	CB-CG	-8.78	1.33	1.51
1	A	671	ARG	CZ-NH1	7.88	1.43	1.33
1	A	333	THR	N-CA	7.78	1.61	1.46
1	A	524	SER	CB-OG	-7.68	1.32	1.42
1	A	145	PHE	CE1-CZ	7.18	1.50	1.37

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ASP	CB-CG-OD1	-27.14	93.87	118.30
1	A	421	ASP	CB-CG-OD2	19.82	136.13	118.30
1	A	410	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	A	671	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	A	810	ARG	NE-CZ-NH2	-12.48	114.06	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide
1	A	145	PHE	Mainchain
1	A	637	GLY	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	5325	0	5038	53	0
2	A	40	0	41	10	0
3	A	253	0	368	7	0
4	A	48	0	64	1	0
5	A	20	0	0	0	0
6	A	2	0	0	0	0
7	A	257	0	0	6	0
All	All	5945	0	5511	62	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 6.

The worst 5 of 62 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)
2:A:901:0UE:N31	2:A:901:0UE:C31	1.70	1.51
2:A:901:0UE:C21	2:A:901:0UE:N21	1.81	1.44
2:A:901:0UE:N11	2:A:901:0UE:C11	1.85	1.39
1:A:757:ARG:HH22	3:A:913:BNG:H2	1.39	0.86
2:A:901:0UE:C21	2:A:901:0UE:C19	2.52	0.85

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	675/677 (100%)	652 (97%)	22 (3%)	1 (0%)	48 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE

### 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	566/566 (100%)	534 (94%)	32 (6%)	17 5

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	748	THR
1	A	768	ILE
1	A	393	ARG
1	A	389	ARG
1	A	777	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	653	ASN
1	A	682	GLN
1	A	385	HIS
1	A	374	HIS

### 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 ⓘ

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 for Mogul analysis.

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	$\# Z  > 2$
3	BNG	A	902	-	11,11,21	0.57	0	9,10,26	0.21	0
3	BNG	A	906	-	21,21,21	0.76	1 (4%)	26,26,26	1.51	4 (15%)
3	BNG	A	912	-	21,21,21	0.86	1 (4%)	26,26,26	1.36	4 (15%)
2	0UE	A	901	-	44,44,44	10.11	26 (59%)	44,66,66	8.69	27 (61%)
3	BNG	A	905	-	21,21,21	0.98	1 (4%)	26,26,26	1.81	6 (23%)
3	BNG	A	907	-	21,21,21	0.71	1 (4%)	26,26,26	1.48	4 (15%)
5	SO4	A	925	-	4,4,4	0.59	0	6,6,6	0.34	0
3	BNG	A	909	-	21,21,21	0.86	1 (4%)	26,26,26	1.30	3 (11%)
3	BNG	A	910	-	9,9,21	0.28	0	8,8,26	0.73	0
4	GOL	A	917	-	5,5,5	0.24	0	5,5,5	0.65	0
4	GOL	A	919	-	5,5,5	0.27	0	5,5,5	0.55	0
3	BNG	A	908	-	21,21,21	0.62	0	26,26,26	0.99	2 (7%)
4	GOL	A	921	-	5,5,5	0.85	0	5,5,5	1.62	2 (40%)
4	GOL	A	918	-	5,5,5	0.36	0	5,5,5	0.74	0
5	SO4	A	923	-	4,4,4	0.59	0	6,6,6	0.48	0
3	BNG	A	904	-	21,21,21	0.67	0	26,26,26	1.11	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	924	-	4,4,4	1.31	1 (25%)	6,6,6	0.68	0
4	GOL	A	916	-	5,5,5	0.64	0	5,5,5	1.51	0
4	GOL	A	915	-	5,5,5	0.39	0	5,5,5	0.81	0
4	GOL	A	922	-	5,5,5	0.73	0	5,5,5	0.85	0
3	BNG	A	911	-	21,21,21	1.12	1 (4%)	26,26,26	1.44	3 (11%)
3	BNG	A	913	-	21,21,21	1.45	3 (14%)	26,26,26	3.24	7 (26%)
4	GOL	A	920	-	5,5,5	1.05	0	5,5,5	0.88	0
3	BNG	A	914	-	21,21,21	0.54	0	26,26,26	1.20	3 (11%)
5	SO4	A	926	-	4,4,4	0.43	0	6,6,6	0.38	0
3	BNG	A	903	-	21,21,21	0.98	1 (4%)	26,26,26	1.62	3 (11%)

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
3	BNG	A	902	-	-	3/8/9/32	-
3	BNG	A	906	-	-	11/12/32/32	0/1/1/1
3	BNG	A	912	-	-	9/12/32/32	0/1/1/1
2	0UE	A	901	-	1/1/9/11	12/34/88/88	0/3/5/5
3	BNG	A	905	-	-	7/12/32/32	0/1/1/1
3	BNG	A	907	-	-	3/12/32/32	0/1/1/1
3	BNG	A	909	-	-	6/12/32/32	0/1/1/1
3	BNG	A	910	-	-	3/7/7/32	-
4	GOL	A	917	-	-	2/4/4/4	-
4	GOL	A	919	-	-	0/4/4/4	-
3	BNG	A	908	-	-	9/12/32/32	0/1/1/1
4	GOL	A	921	-	-	0/4/4/4	-
4	GOL	A	918	-	-	2/4/4/4	-
3	BNG	A	904	-	-	8/12/32/32	0/1/1/1
4	GOL	A	916	-	-	3/4/4/4	-
4	GOL	A	915	-	-	0/4/4/4	-
4	GOL	A	922	-	-	0/4/4/4	-
3	BNG	A	911	-	-	2/12/32/32	0/1/1/1
3	BNG	A	913	-	-	4/12/32/32	0/1/1/1
4	GOL	A	920	-	-	4/4/4/4	-
3	BNG	A	914	-	-	5/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BNG	A	903	-	-	5/12/32/32	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	0UE	C11-N11	34.07	1.85	1.31
2	A	901	0UE	C21-N21	31.59	1.81	1.31
2	A	901	0UE	C39-N11	-25.61	1.02	1.47
2	A	901	0UE	C19-N21	-23.93	1.05	1.47
2	A	901	0UE	O22-C21	14.53	1.52	1.28

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	0UE	O21-N21-C21	-37.33	92.03	116.42
2	A	901	0UE	O11-N11-C11	-21.34	102.48	116.42
2	A	901	0UE	O22-C21-N21	-19.23	103.71	118.38
2	A	901	0UE	O22-C21-C22	16.72	137.74	120.13
2	A	901	0UE	O12-C11-N11	-13.95	107.73	118.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	0UE	N31

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	0UE	O12-C11-C12-C13
2	A	901	0UE	N11-C11-C12-C13
2	A	901	0UE	C17-C18-C19-N21
2	A	901	0UE	C18-C19-N21-C21
2	A	901	0UE	N11-C39-C40-C41

There are no ring outliers.

7 monomers are involved in 18 short contacts:

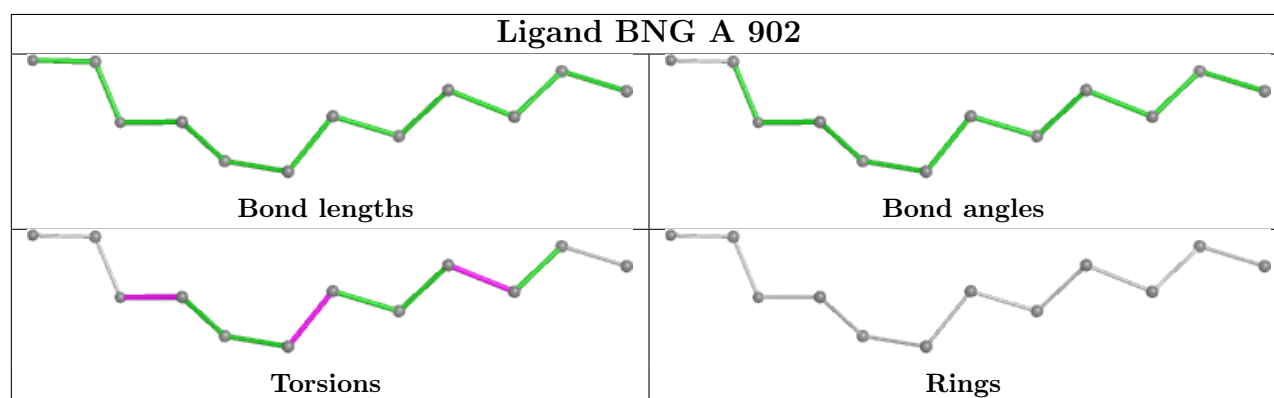
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	906	BNG	2	0
2	A	901	0UE	10	0
3	A	905	BNG	1	0

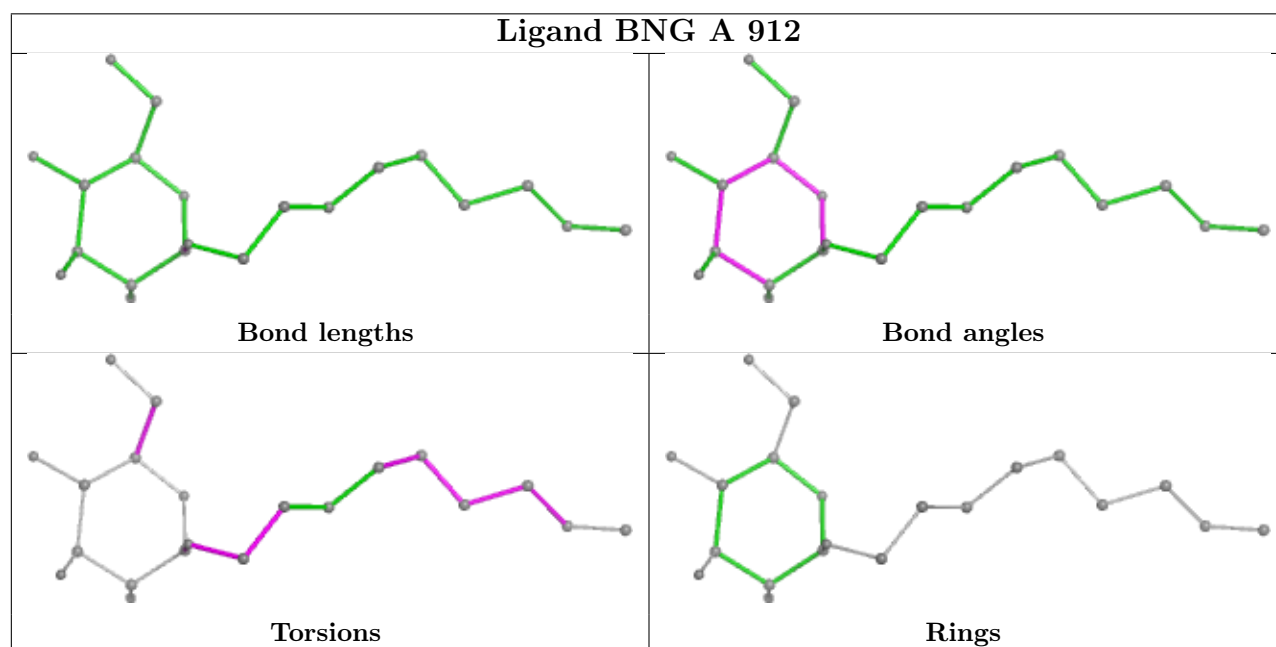
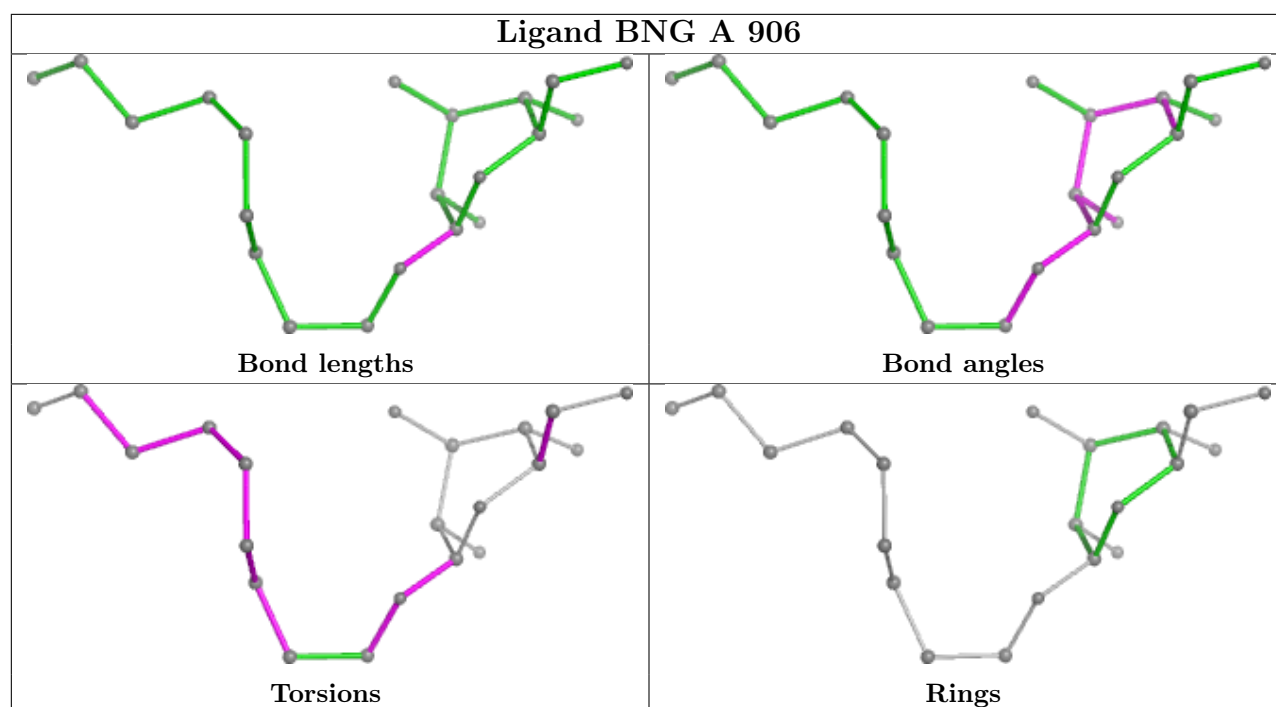
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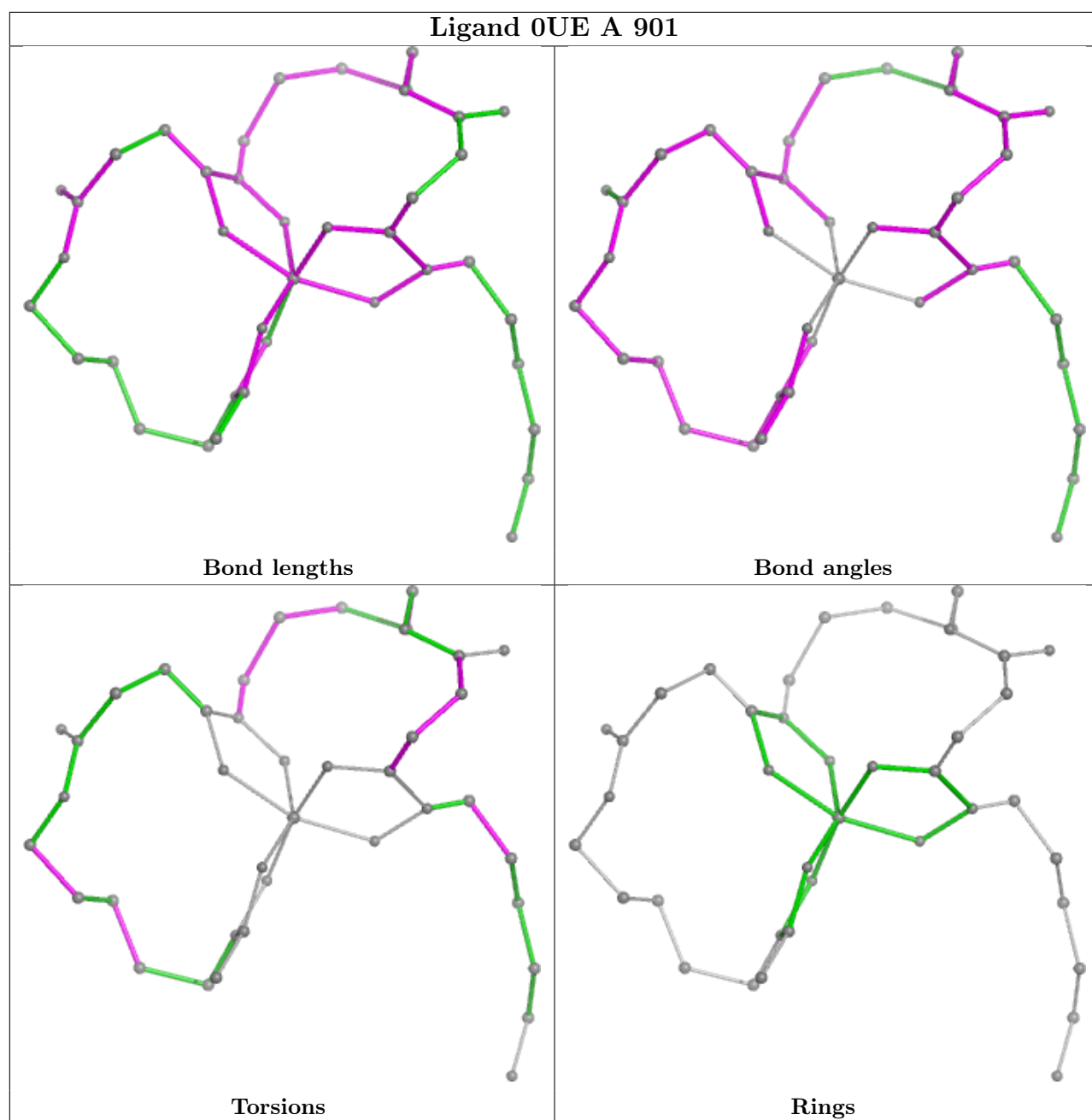
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	BNG	1	0
3	A	911	BNG	1	0
3	A	913	BNG	2	0
4	A	920	GOL	1	0

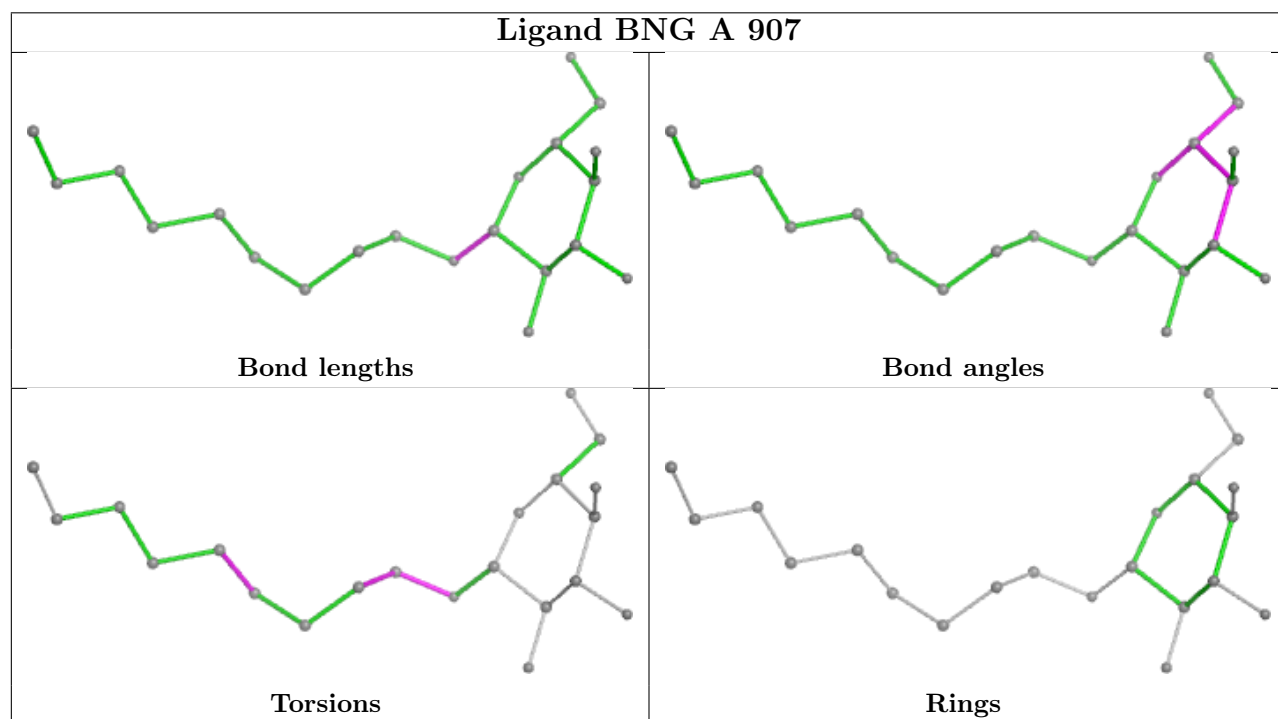
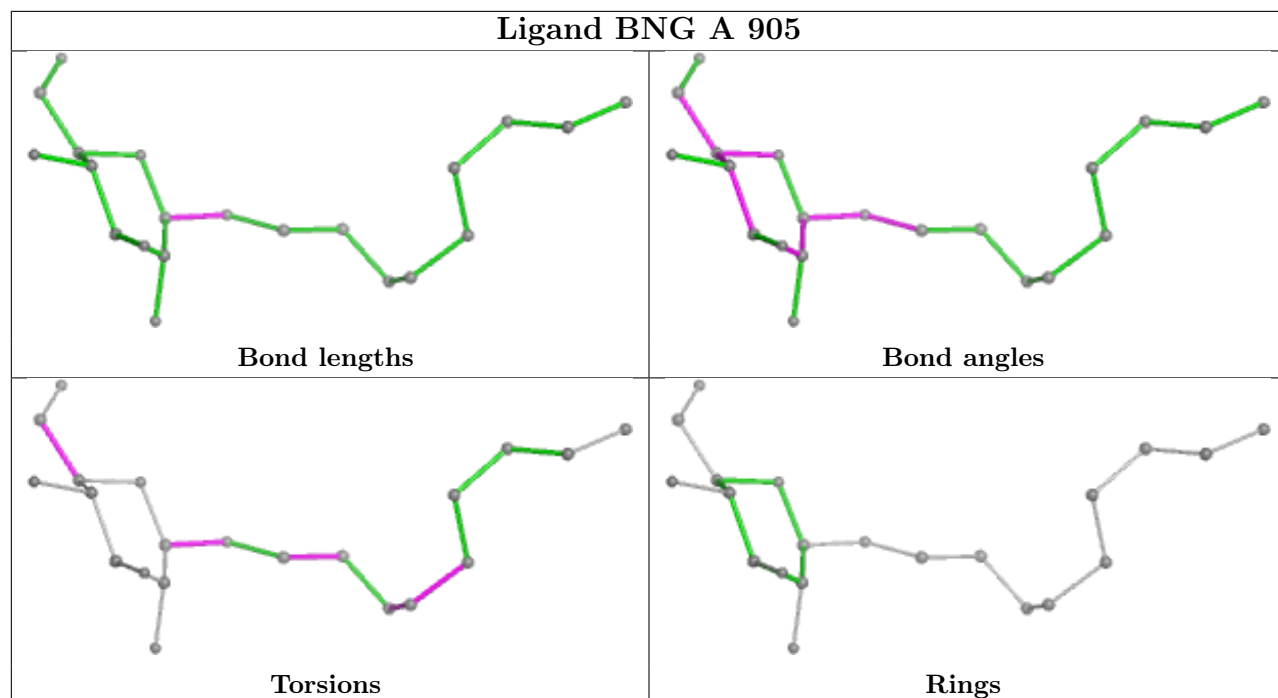
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

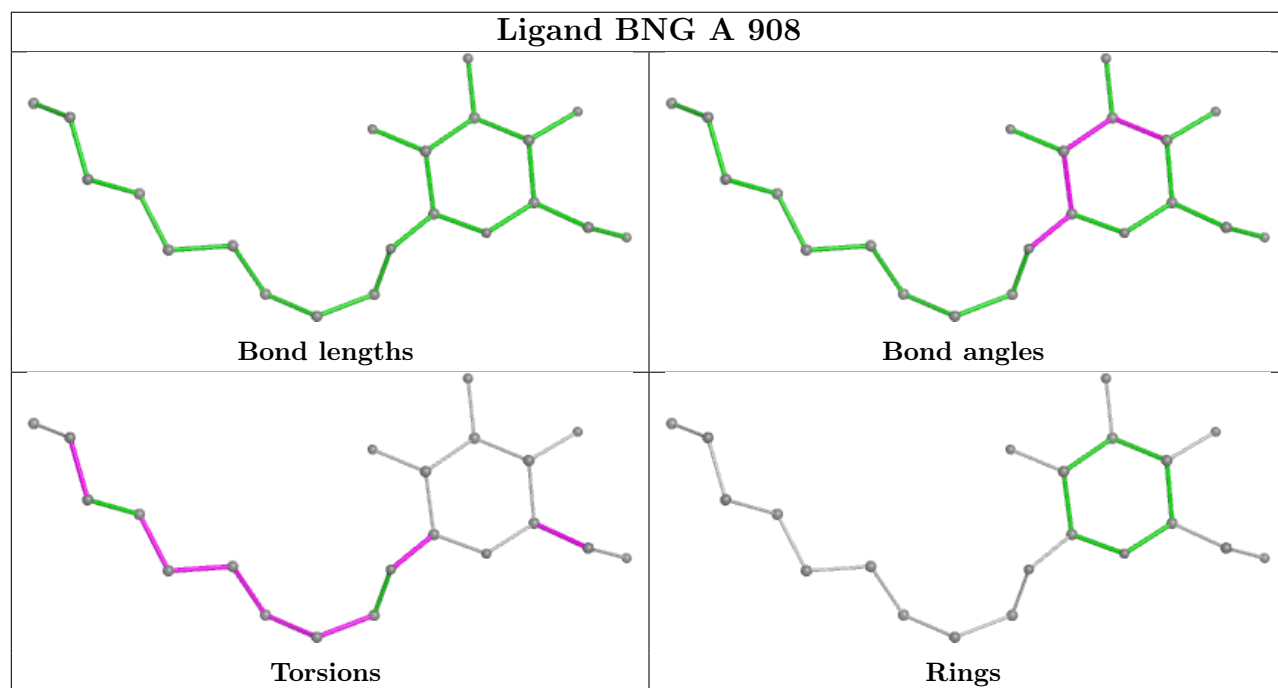
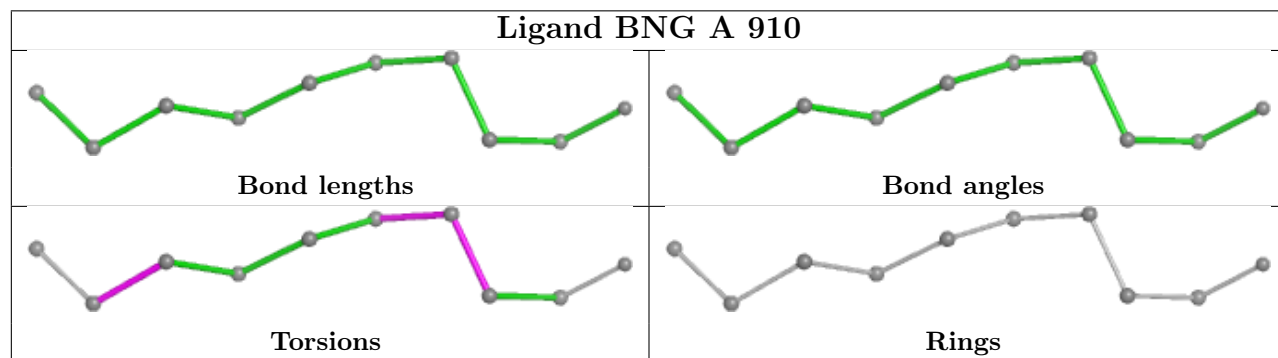
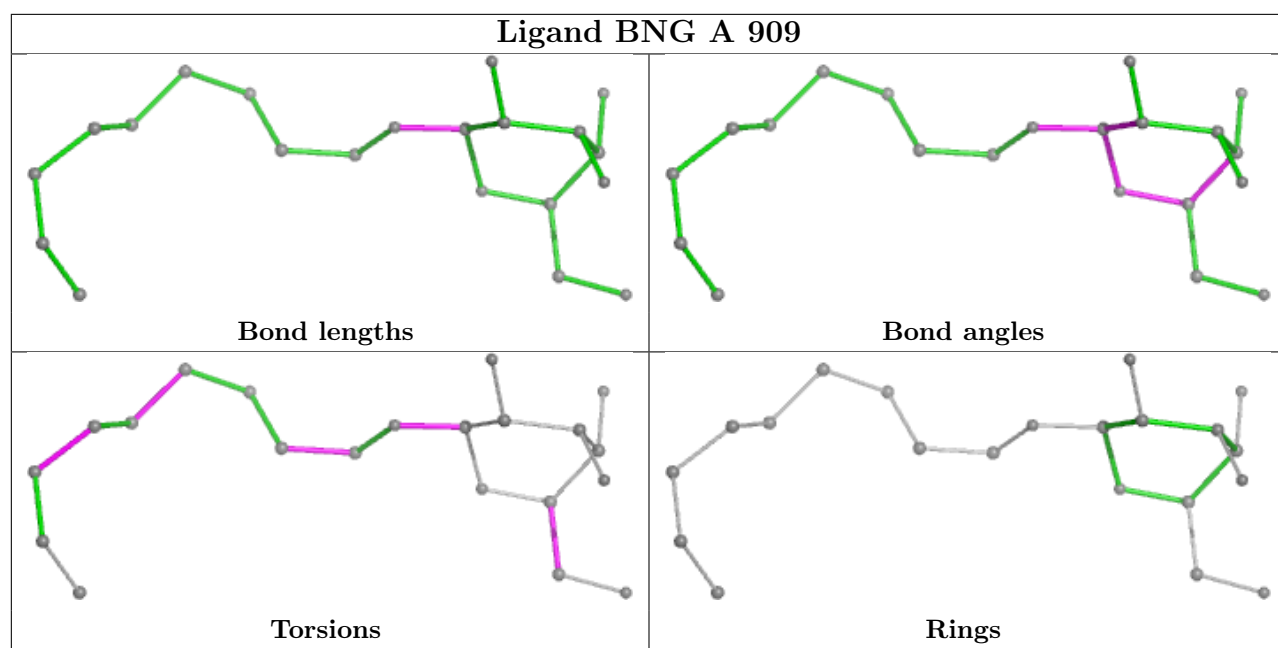


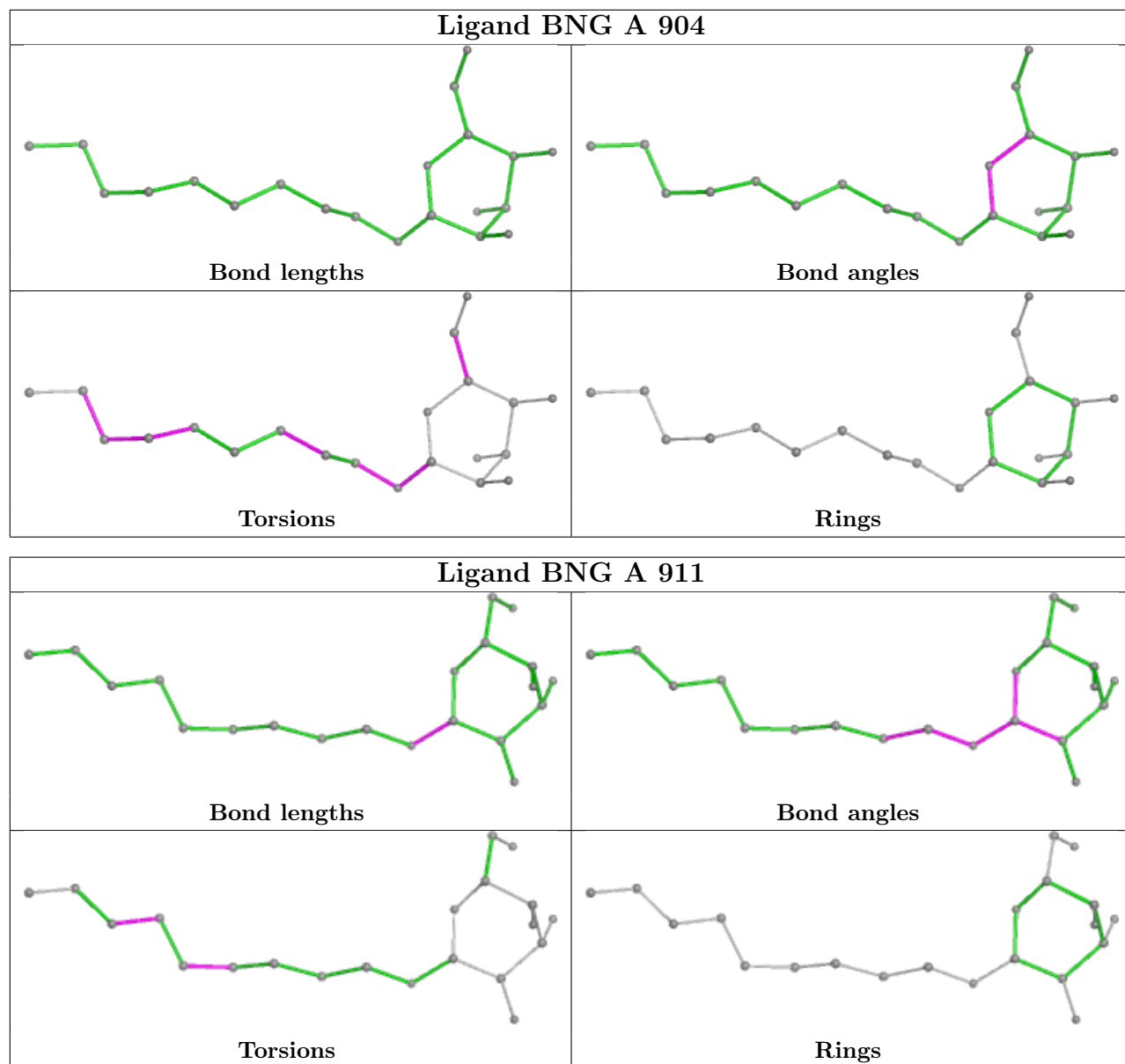


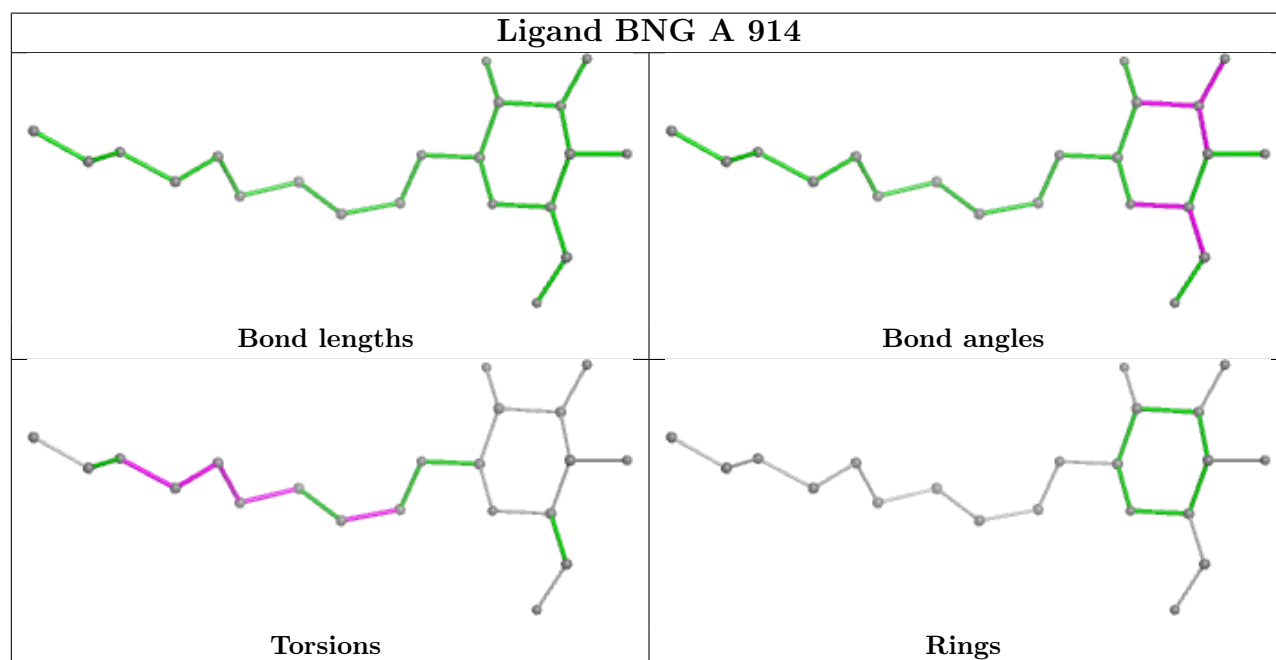
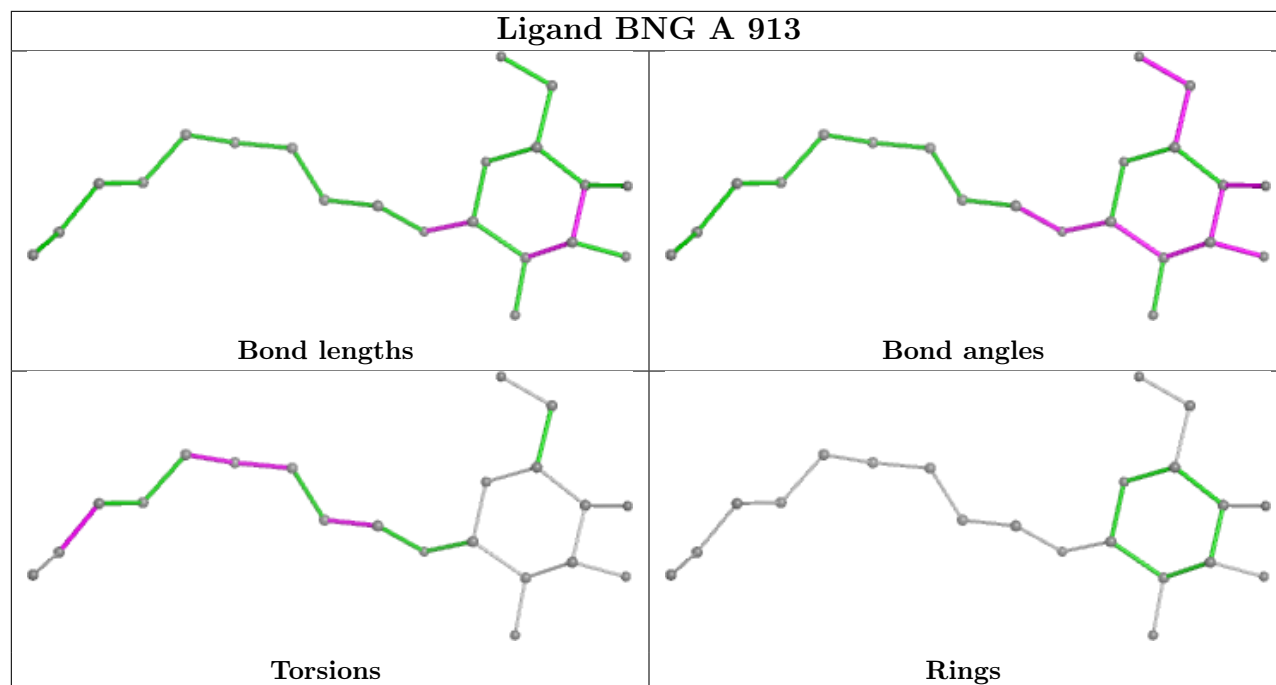


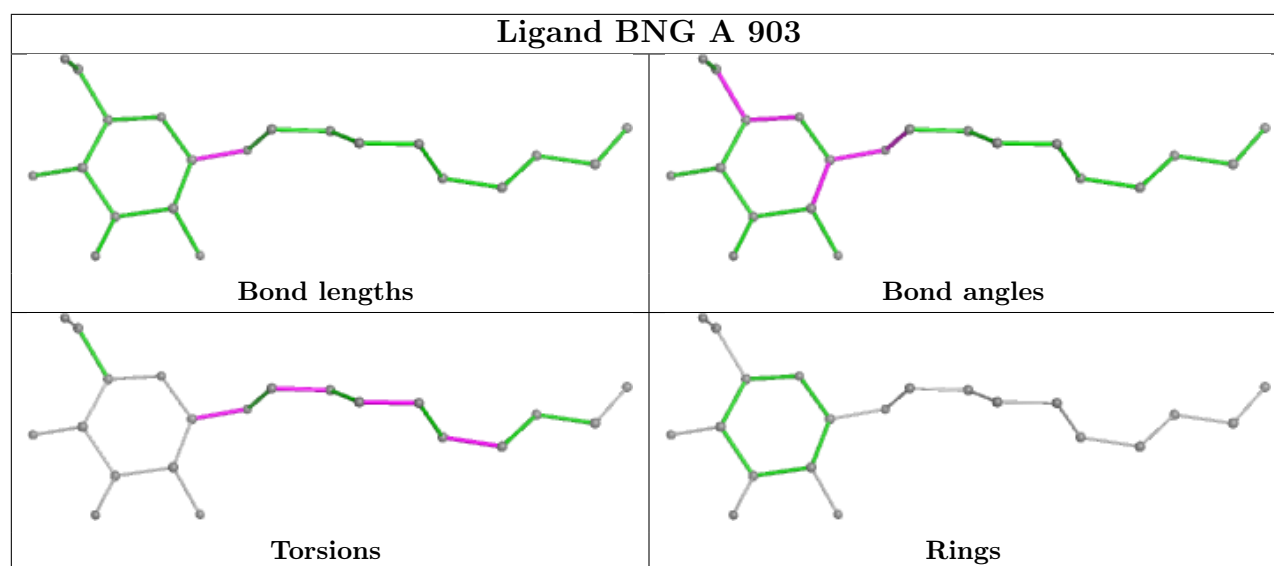












## 5.7 Other polymers [i](#)

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	677/677 (100%)	0.17	31 (4%) 38 40	29, 45, 78, 112	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	6.0
1	A	144	VAL	5.9
1	A	614	ALA	4.8
1	A	777	LEU	3.7
1	A	663	PHE	3.5

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	925	5/5	0.51	0.18	104,105,118,118	0
5	SO4	A	926	5/5	0.59	0.11	99,113,117,120	0

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*Continued from previous page...*

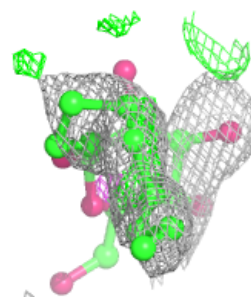
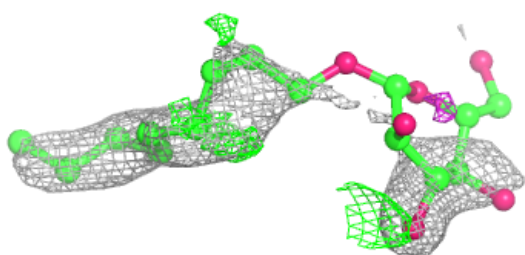
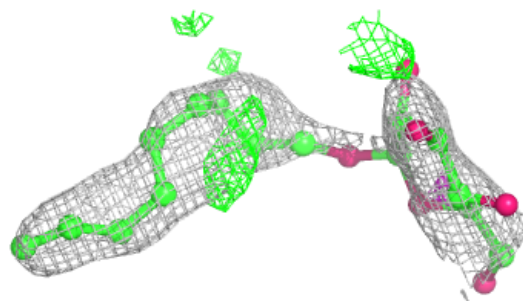
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	923	5/5	0.72	0.13	77,95,110,113	0
3	BNG	A	905	21/21	0.74	0.24	61,102,119,131	0
3	BNG	A	913	21/21	0.76	0.23	51,77,88,99	0
4	GOL	A	916	6/6	0.77	0.20	54,64,73,99	0
4	GOL	A	917	6/6	0.78	0.16	77,87,98,102	0
3	BNG	A	904	21/21	0.79	0.25	53,76,98,104	0
3	BNG	A	906	21/21	0.79	0.21	61,78,121,127	0
4	GOL	A	922	6/6	0.80	0.17	72,84,86,89	0
3	BNG	A	908	21/21	0.80	0.24	61,87,98,102	0
3	BNG	A	911	21/21	0.82	0.23	55,77,96,103	0
3	BNG	A	909	21/21	0.83	0.20	64,89,115,118	0
3	BNG	A	912	21/21	0.83	0.18	67,107,133,135	0
3	BNG	A	910	10/21	0.83	0.26	72,78,90,93	0
3	BNG	A	903	21/21	0.84	0.17	64,80,100,111	0
3	BNG	A	902	12/21	0.84	0.27	70,81,105,106	0
3	BNG	A	914	21/21	0.84	0.15	65,83,99,102	0
3	BNG	A	907	21/21	0.85	0.15	60,109,127,129	0
4	GOL	A	919	6/6	0.85	0.14	45,79,89,92	0
4	GOL	A	920	6/6	0.87	0.15	57,61,66,70	0
6	NA	A	928	1/1	0.89	0.41	76,76,76,76	0
4	GOL	A	921	6/6	0.91	0.14	47,56,66,68	0
5	SO4	A	924	5/5	0.93	0.09	42,46,56,59	0
4	GOL	A	918	6/6	0.94	0.09	43,49,51,54	0
2	OUE	A	901	40/40	0.94	0.14	37,47,66,68	0
6	NA	A	927	1/1	0.96	0.08	42,42,42,42	0
4	GOL	A	915	6/6	0.97	0.06	31,34,36,38	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.

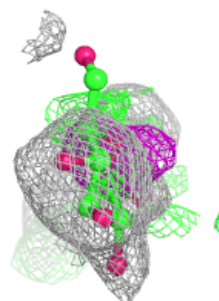
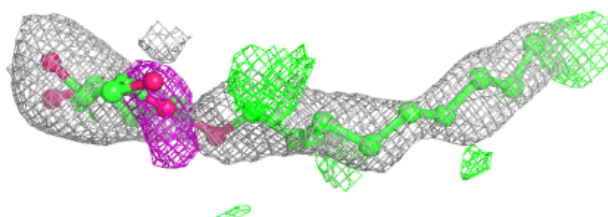
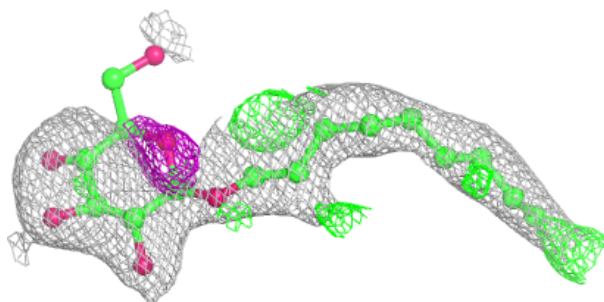


**Electron density around BNG A 905:**

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

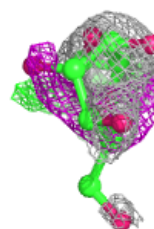
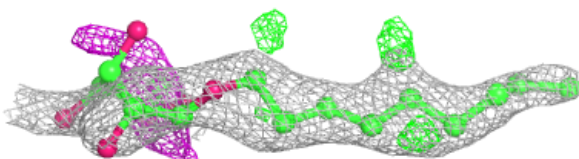
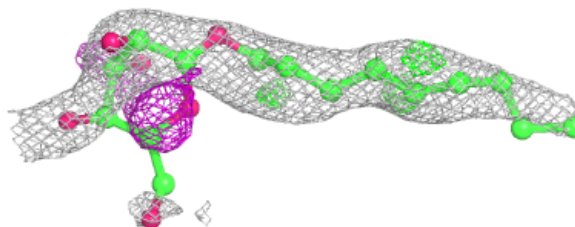
**Electron density around BNG A 913:**

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and green (positive)

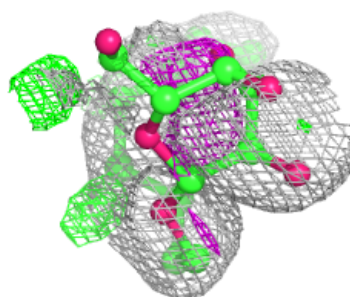
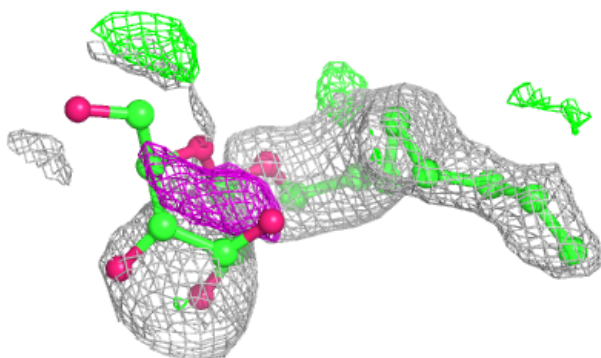
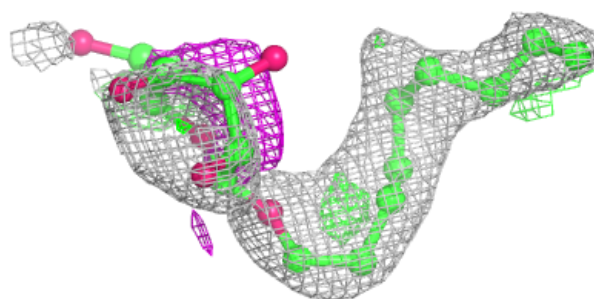


**Electron density around BNG A 904:**

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and green (positive)

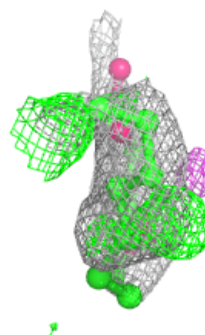
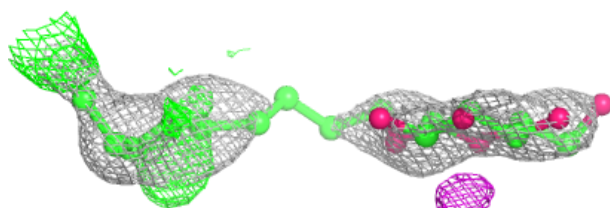
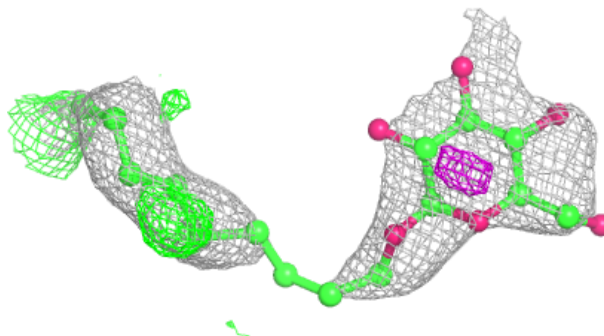
**Electron density around BNG A 906:**

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

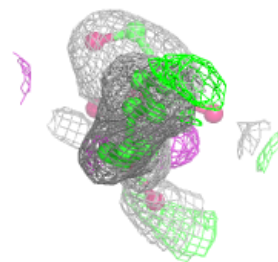
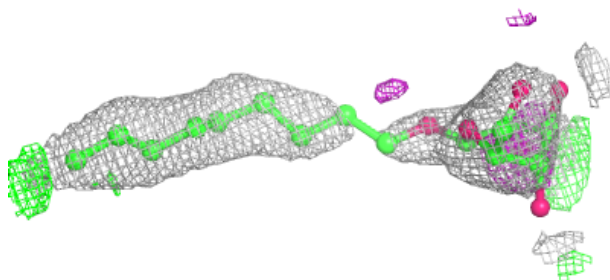
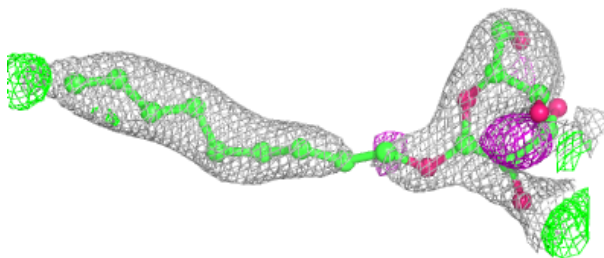


**Electron density around BNG A 908:**

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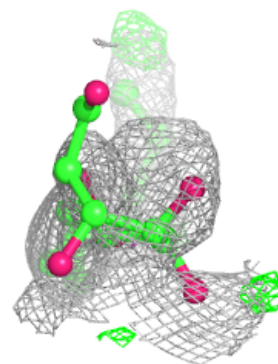
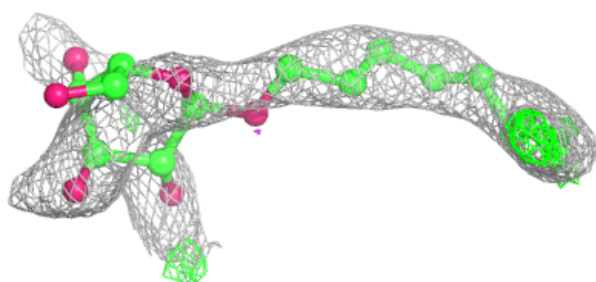
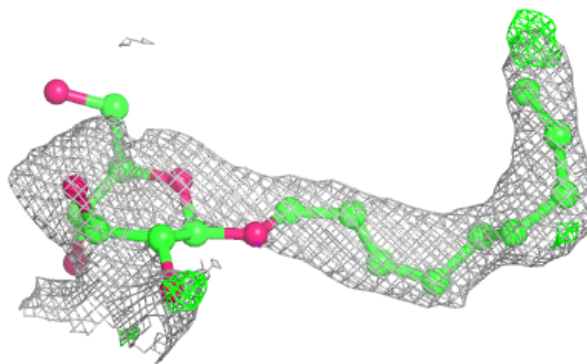
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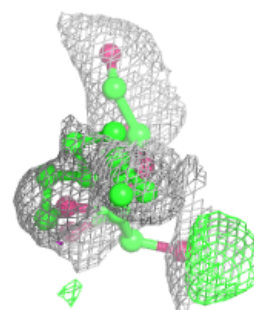
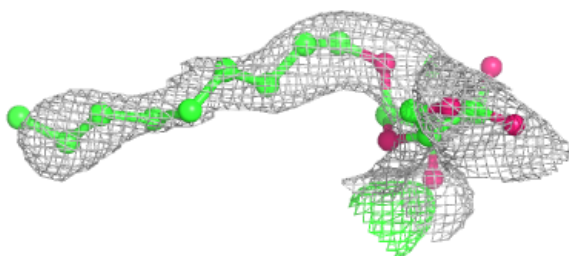
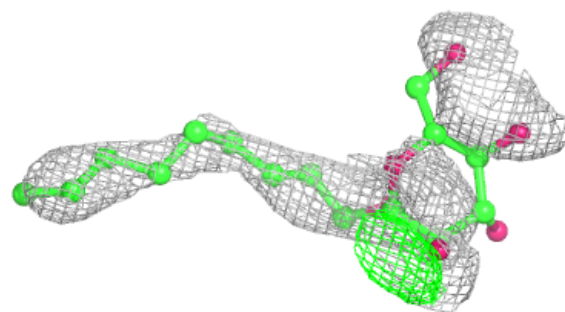


**Electron density around BNG A 909:**

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

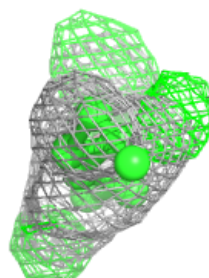
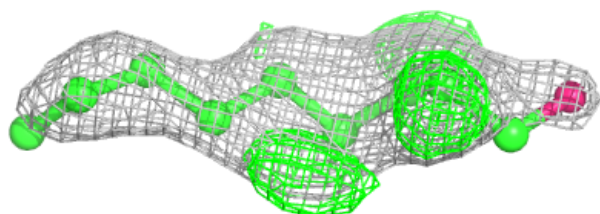
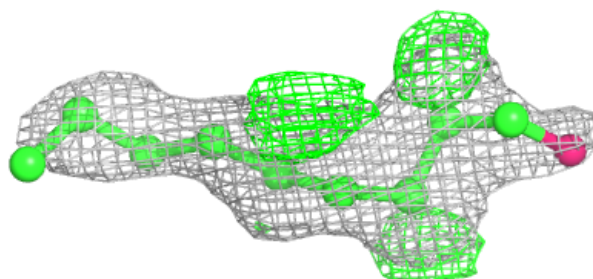
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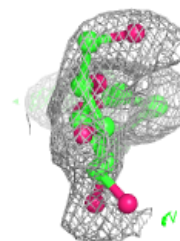
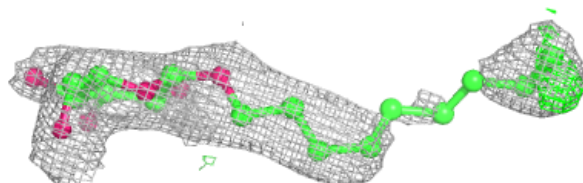
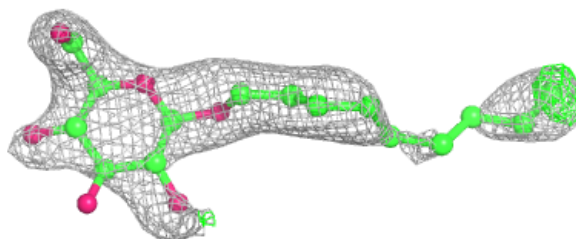


**Electron density around BNG A 910:**

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and green (positive)

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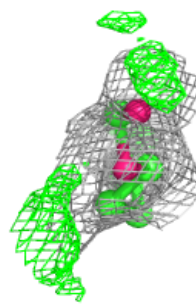
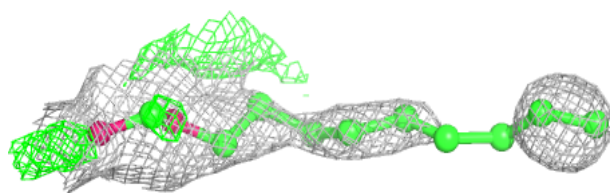
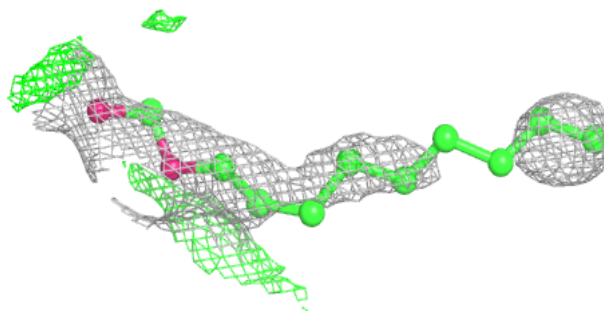
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



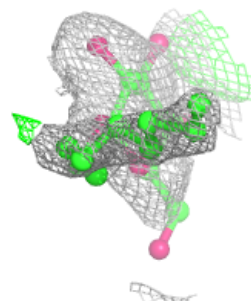
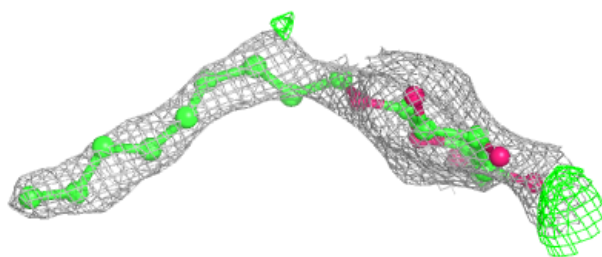
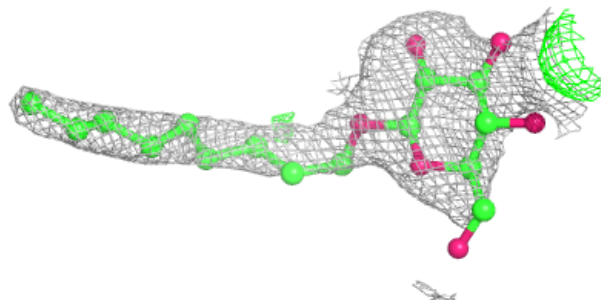


**Electron density around BNG A 902:**

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

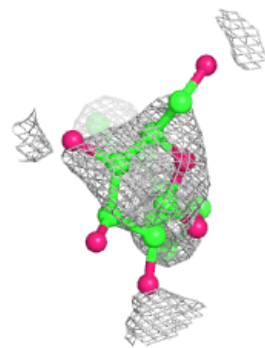
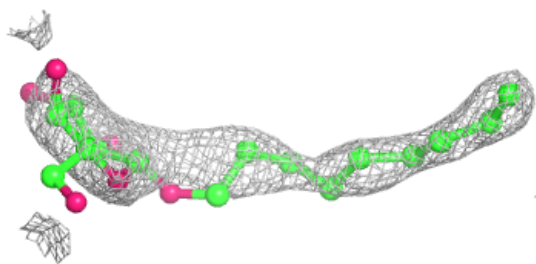
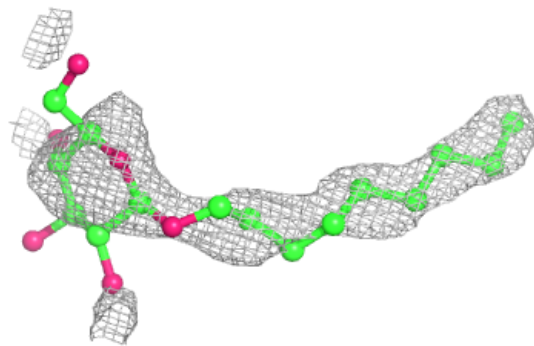
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and green (positive)



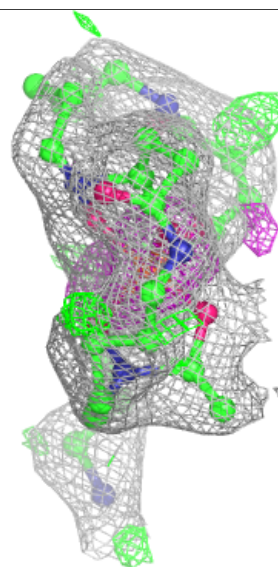
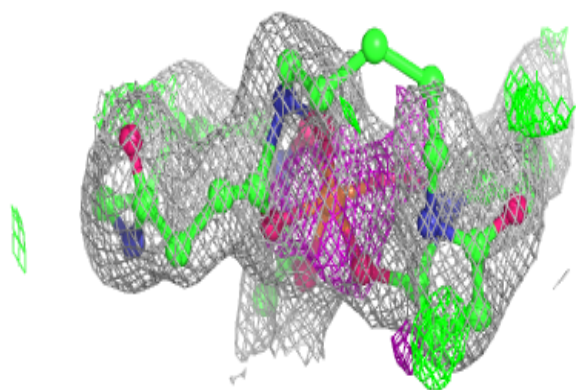
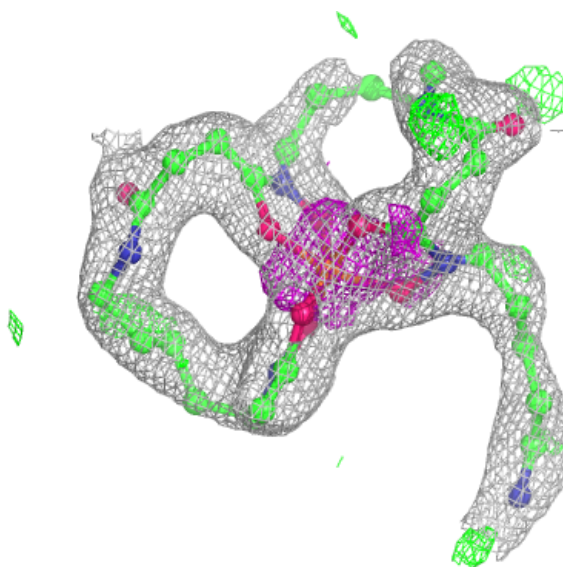
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$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



**Electron density around OUE A 901:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.