



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:56 AM BST

PDB ID : 6FFV
Title : The crystal structure of BtuM cobalamin transporter
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Deposited on : 2018-01-09
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

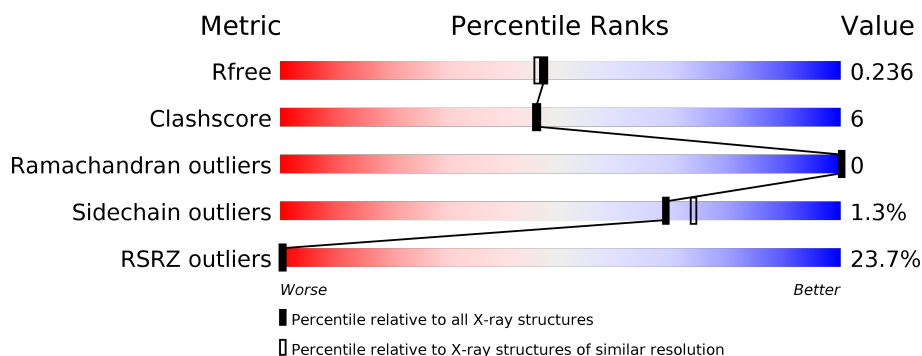
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	207	<div> <div>22%</div> <div>85%</div> <div>9%</div> <div>6%</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
3	PG4	A	302	-	-	-	X
4	BNG	A	308	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 1863 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.

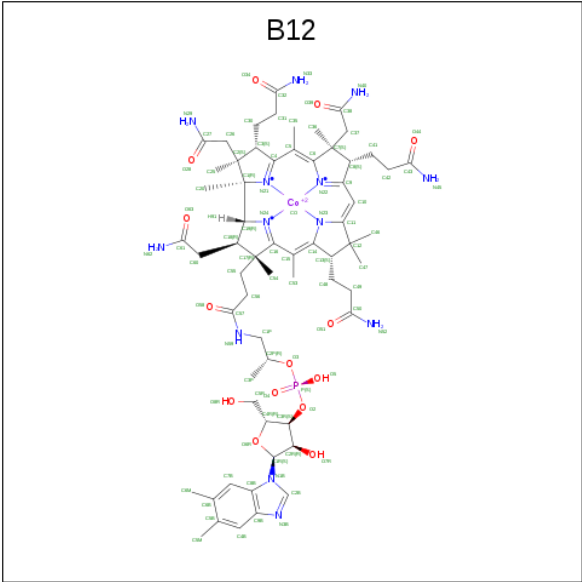
- Molecule 1 is a protein called BtuM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	4	0
			1557	1038	274	239	6			

There are 10 discrepancies between the modelled and reference sequences:

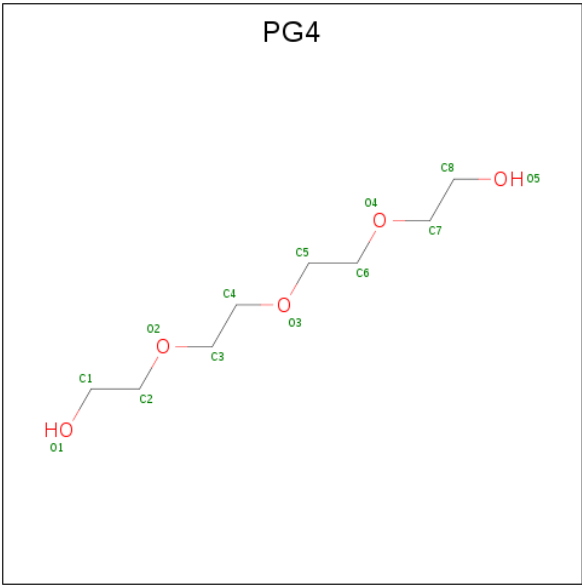
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q3SFD8
A	2	GLY	-	cloning artifact	UNP Q3SFD8
A	200	HIS	-	expression tag	UNP Q3SFD8
A	201	HIS	-	expression tag	UNP Q3SFD8
A	202	HIS	-	expression tag	UNP Q3SFD8
A	203	HIS	-	expression tag	UNP Q3SFD8
A	204	HIS	-	expression tag	UNP Q3SFD8
A	205	HIS	-	expression tag	UNP Q3SFD8
A	206	HIS	-	expression tag	UNP Q3SFD8
A	207	HIS	-	expression tag	UNP Q3SFD8

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



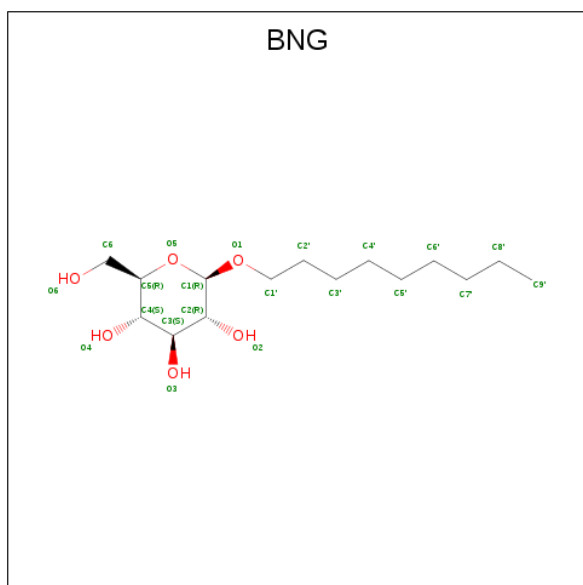
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	8	5	0	0
3	A	1	13	8	5	0	0
3	A	1	13	8	5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

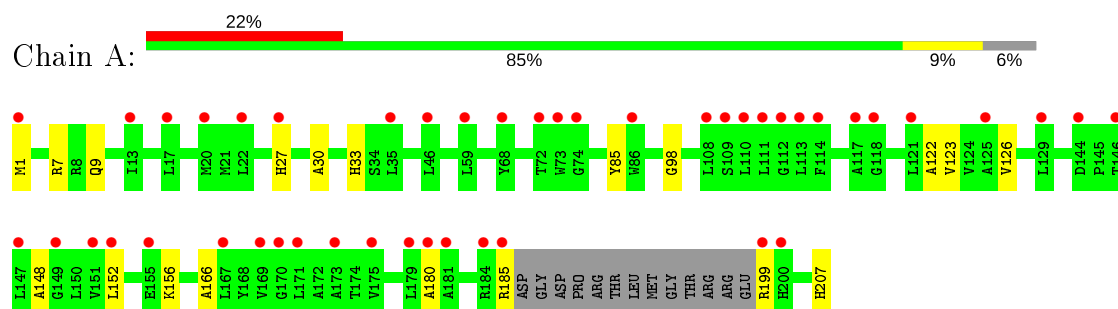
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		

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: BtuM



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.54Å 87.54Å 97.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.77 – 2.01 43.77 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.77-2.01) 98.6 (43.77-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.202 , 0.236 0.202 , 0.236	Depositor DCC
R_{free} test set	1449 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1863	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, BNG, PG4, PGE, B12

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	0.42	0/1611	0.56	0/2196

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1557	0	1585	14	0
2	A	91	0	87	11	0
3	A	65	0	90	2	0
4	A	63	0	90	4	0
5	A	49	0	70	0	0
6	A	10	0	14	0	0
7	A	28	0	0	2	0
All	All	1863	0	1936	24	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.

All (24) 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:301:B12:H401	2:A:301:B12:H8	1.62	0.64
4:A:308:BNG:H9'2	4:A:309:BNG:H9'3	1.81	0.62
1:A:27[A]:HIS:H	2:A:301:B12:H452	1.46	0.60
1:A:27[B]:HIS:H	2:A:301:B12:H452	1.47	0.60
2:A:301:B12:H371	2:A:301:B12:H351	1.84	0.60
1:A:180:ALA:HA	4:A:307:BNG:H1	1.83	0.60
1:A:7:ARG:HH12	3:A:303:PG4:H72	1.67	0.59
1:A:156:LYS:NZ	7:A:402:HOH:O	2.37	0.57
1:A:98:GLY:HA3	1:A:123:VAL:HG11	1.91	0.53
1:A:207:HIS:HD2	7:A:404:HOH:O	1.92	0.51
1:A:148:ALA:O	1:A:152:LEU:HD23	2.14	0.47
1:A:122:ALA:O	1:A:126:VAL:HG13	2.14	0.47
1:A:30:ALA:HA	1:A:33:HIS:CE1	2.49	0.47
2:A:301:B12:C37	2:A:301:B12:H351	2.46	0.46
1:A:9:GLN:HG2	4:A:309:BNG:H3'2	1.99	0.44
1:A:85:TYR:HA	2:A:301:B12:N33	2.33	0.43
2:A:301:B12:H531	2:A:301:B12:H552	1.99	0.43
2:A:301:B12:O28	2:A:301:B12:H3	2.17	0.43
4:A:309:BNG:H2'1	4:A:309:BNG:H5'1	1.86	0.42
1:A:166:ALA:HB1	3:A:305:PG4:H61	2.02	0.41
2:A:301:B12:H541	2:A:301:B12:H602	1.89	0.41
2:A:301:B12:H2B	2:A:301:B12:O2	2.20	0.41
1:A:199:ARG:NE	1:A:199:ARG:HA	2.36	0.40
2:A:301:B12:H481	2:A:301:B12:H473	1.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/207 (94%)	193 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	155/162 (96%)	153 (99%)	2 (1%)	69 74

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
3	PG4	A	302	-	12,12,12	0.51	0	11,11,11	0.17	0
5	PEG	A	316	-	6,6,6	0.49	0	5,5,5	0.27	0
3	PG4	A	303	-	12,12,12	0.51	0	11,11,11	0.44	0
5	PEG	A	312	-	6,6,6	0.44	0	5,5,5	0.24	0
3	PG4	A	304	-	12,12,12	0.50	0	11,11,11	0.24	0
5	PEG	A	311	-	6,6,6	0.49	0	5,5,5	0.29	0
5	PEG	A	313	-	6,6,6	0.49	0	5,5,5	0.48	0
4	BNG	A	307	-	21,21,21	1.12	1 (4%)	26,26,26	1.54	5 (19%)
5	PEG	A	314	-	6,6,6	0.47	0	5,5,5	0.36	0
3	PG4	A	305	-	12,12,12	0.52	0	11,11,11	0.31	0
5	PEG	A	310	-	6,6,6	0.48	0	5,5,5	0.28	0
6	PGE	A	317	-	9,9,9	0.29	0	8,8,8	0.38	0
4	BNG	A	308	-	21,21,21	1.15	2 (9%)	26,26,26	0.77	0
4	BNG	A	309	-	21,21,21	1.16	2 (9%)	26,26,26	1.28	3 (11%)
3	PG4	A	306	-	12,12,12	0.53	0	11,11,11	0.19	0
5	PEG	A	315	-	6,6,6	0.49	0	5,5,5	0.23	0
2	B12	A	301	-	80,101,101	1.11	6 (7%)	101,166,166	2.35	18 (17%)

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	PG4	A	302	-	-	6/10/10/10	-
5	PEG	A	316	-	-	3/4/4/4	-
3	PG4	A	303	-	-	7/10/10/10	-
5	PEG	A	312	-	-	1/4/4/4	-
3	PG4	A	304	-	-	3/10/10/10	-
5	PEG	A	311	-	-	1/4/4/4	-
5	PEG	A	313	-	-	3/4/4/4	-
4	BNG	A	307	-	-	4/12/32/32	0/1/1/1
5	PEG	A	314	-	-	2/4/4/4	-
3	PG4	A	305	-	-	4/10/10/10	-
5	PEG	A	310	-	-	2/4/4/4	-
6	PGE	A	317	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BNG	A	308	-	-	8/12/32/32	0/1/1/1
4	BNG	A	309	-	-	4/12/32/32	0/1/1/1
3	PG4	A	306	-	-	6/10/10/10	-
5	PEG	A	315	-	-	1/4/4/4	-
2	B12	A	301	-	-	14/51/223/223	0/3/11/11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	B12	C11-C10	-4.52	1.33	1.40
2	A	301	B12	C8B-C9B	3.75	1.48	1.40
4	A	307	BNG	O5-C1	3.71	1.51	1.41
4	A	308	BNG	O5-C1	3.56	1.50	1.41
4	A	309	BNG	O5-C1	3.44	1.50	1.41
2	A	301	B12	C6B-C5B	2.99	1.48	1.40
2	A	301	B12	C2-C3	-2.39	1.54	1.58
4	A	309	BNG	O1-C1	-2.38	1.36	1.40
2	A	301	B12	C14-C15	2.30	1.48	1.40
4	A	308	BNG	O1-C1	-2.29	1.36	1.40
2	A	301	B12	C17-C18	2.17	1.57	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	B12	C20-C1-C19	-13.41	96.43	109.36
2	A	301	B12	C19-C1-N21	8.31	110.67	102.16
2	A	301	B12	C1-C19-C18	7.41	134.18	121.93
2	A	301	B12	C12-C11-C10	-5.70	114.97	124.64
2	A	301	B12	C2-C1-C19	5.16	126.75	118.60
2	A	301	B12	C47-C12-C46	4.44	119.03	109.73
2	A	301	B12	C26-C2-C1	4.07	116.34	110.02
2	A	301	B12	C8-C9-N22	4.01	116.14	111.12
4	A	307	BNG	C1-C2-C3	3.61	117.51	110.00
4	A	309	BNG	O5-C5-C4	3.60	116.24	109.69
4	A	307	BNG	C4-C3-C2	3.34	116.65	110.82
4	A	307	BNG	C3-C4-C5	3.03	115.65	110.24
2	A	301	B12	C55-C56-C57	-3.00	104.69	111.23
2	A	301	B12	C1-C19-N24	2.98	109.59	106.24
2	A	301	B12	C25-C2-C3	-2.96	111.07	115.58
2	A	301	B12	C60-C18-C19	2.79	121.86	114.62
2	A	301	B12	C16-C15-C14	-2.57	120.27	124.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	B12	C56-C55-C17	-2.56	110.54	115.50
4	A	307	BNG	O1-C1-C2	2.55	112.28	108.30
2	A	301	B12	C37-C7-C6	2.54	118.39	109.92
4	A	309	BNG	C6-C5-C4	-2.53	107.09	113.00
4	A	309	BNG	C3-C4-C5	2.48	114.67	110.24
2	A	301	B12	C6-C5-C4	-2.47	120.42	124.27
2	A	301	B12	C55-C17-C16	2.29	117.55	109.92
2	A	301	B12	C25-C2-C1	-2.22	110.51	113.80
4	A	307	BNG	O5-C1-C2	2.17	114.94	110.35

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	B12	C4-C3-C30-C31
2	A	301	B12	N59-C1P-C2P-O3
3	A	302	PG4	O1-C1-C2-O2
4	A	308	BNG	O5-C5-C6-O6
4	A	308	BNG	C4-C5-C6-O6
4	A	309	BNG	C2'-C3'-C4'-C5'
4	A	309	BNG	O5-C1-O1-C1'
2	A	301	B12	C7-C37-C38-N40
3	A	304	PG4	O3-C5-C6-O4
4	A	307	BNG	O5-C5-C6-O6
3	A	302	PG4	O4-C7-C8-O5
5	A	313	PEG	O1-C1-C2-O2
3	A	306	PG4	O1-C1-C2-O2
4	A	307	BNG	O1-C1'-C2'-C3'
5	A	316	PEG	O2-C3-C4-O4
3	A	303	PG4	O1-C1-C2-O2
5	A	312	PEG	O2-C3-C4-O4
6	A	317	PGE	O1-C1-C2-O2
2	A	301	B12	C7-C37-C38-O39
4	A	309	BNG	O1-C1'-C2'-C3'
2	A	301	B12	C1P-C2P-O3-P
2	A	301	B12	C3P-C2P-O3-P
4	A	308	BNG	C1'-C2'-C3'-C4'
3	A	302	PG4	O2-C3-C4-O3
5	A	314	PEG	O1-C1-C2-O2
5	A	311	PEG	O2-C3-C4-O4
5	A	310	PEG	O1-C1-C2-O2
2	A	301	B12	C41-C42-C43-O44

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Mol	Chain	Res	Type	Atoms
4	A	307	BNG	C1'-C2'-C3'-C4'
3	A	304	PG4	O1-C1-C2-O2
3	A	303	PG4	O2-C3-C4-O3
4	A	308	BNG	O1-C1'-C2'-C3'
3	A	303	PG4	O4-C7-C8-O5
2	A	301	B12	C41-C42-C43-N45
4	A	308	BNG	C3'-C4'-C5'-C6'
5	A	313	PEG	O2-C3-C4-O4
3	A	302	PG4	C3-C4-O3-C5
3	A	305	PG4	C5-C6-O4-C7
3	A	306	PG4	C1-C2-O2-C3
3	A	303	PG4	C5-C6-O4-C7
5	A	313	PEG	C1-C2-O2-C3
3	A	305	PG4	C3-C4-O3-C5
4	A	307	BNG	C4-C5-C6-O6
5	A	316	PEG	O1-C1-C2-O2
6	A	317	PGE	C3-C4-O3-C5
3	A	306	PG4	C4-C3-O2-C2
3	A	302	PG4	O3-C5-C6-O4
3	A	303	PG4	C4-C3-O2-C2
4	A	309	BNG	C1'-C2'-C3'-C4'
2	A	301	B12	N59-C1P-C2P-C3P
2	A	301	B12	C19-C18-C60-C61
5	A	316	PEG	C1-C2-O2-C3
5	A	314	PEG	C1-C2-O2-C3
3	A	306	PG4	C6-C5-O3-C4
4	A	308	BNG	O5-C1-O1-C1'
3	A	305	PG4	O3-C5-C6-O4
3	A	305	PG4	O2-C3-C4-O3
3	A	306	PG4	C8-C7-O4-C6
6	A	317	PGE	C6-C5-O3-C4
3	A	302	PG4	C1-C2-O2-C3
2	A	301	B12	C2-C3-C30-C31
2	A	301	B12	C12-C13-C48-C49
3	A	303	PG4	O3-C5-C6-O4
4	A	308	BNG	C2'-C3'-C4'-C5'
6	A	317	PGE	C4-C3-O2-C2
4	A	308	BNG	C6'-C7'-C8'-C9'
5	A	310	PEG	O2-C3-C4-O4
5	A	315	PEG	O2-C3-C4-O4
2	A	301	B12	C2P-O3-P-O2
3	A	306	PG4	C5-C6-O4-C7

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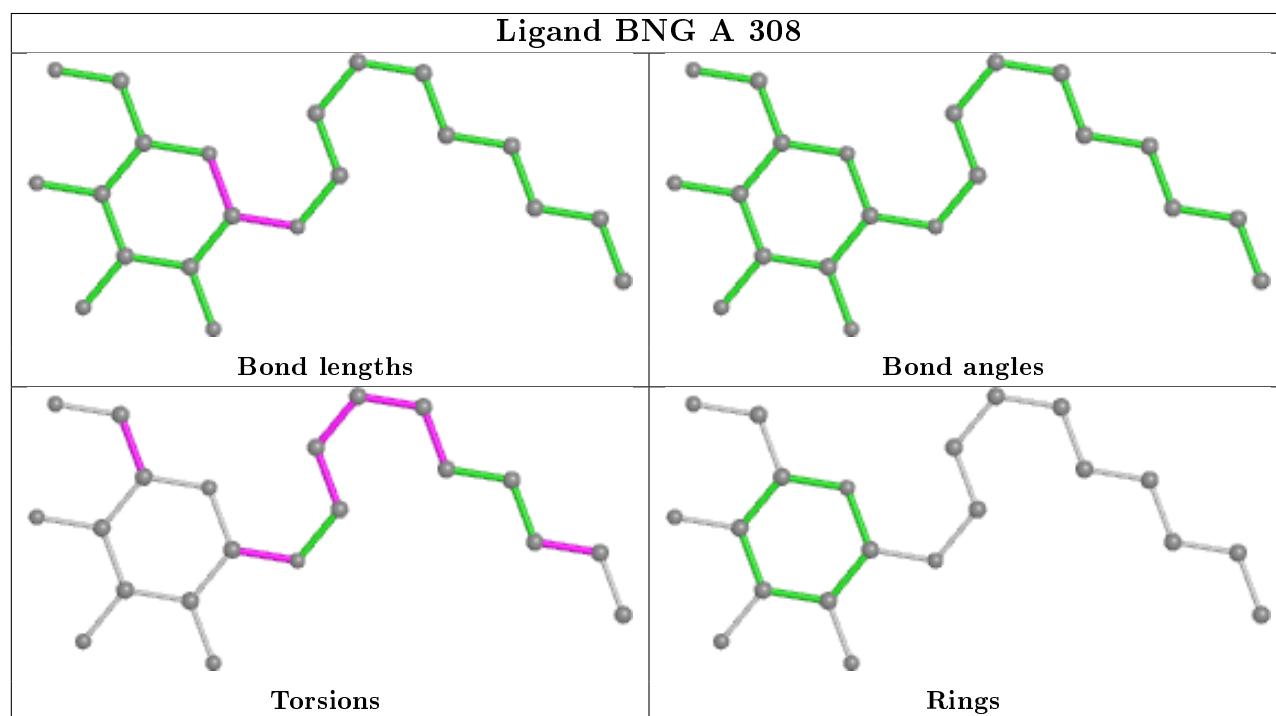
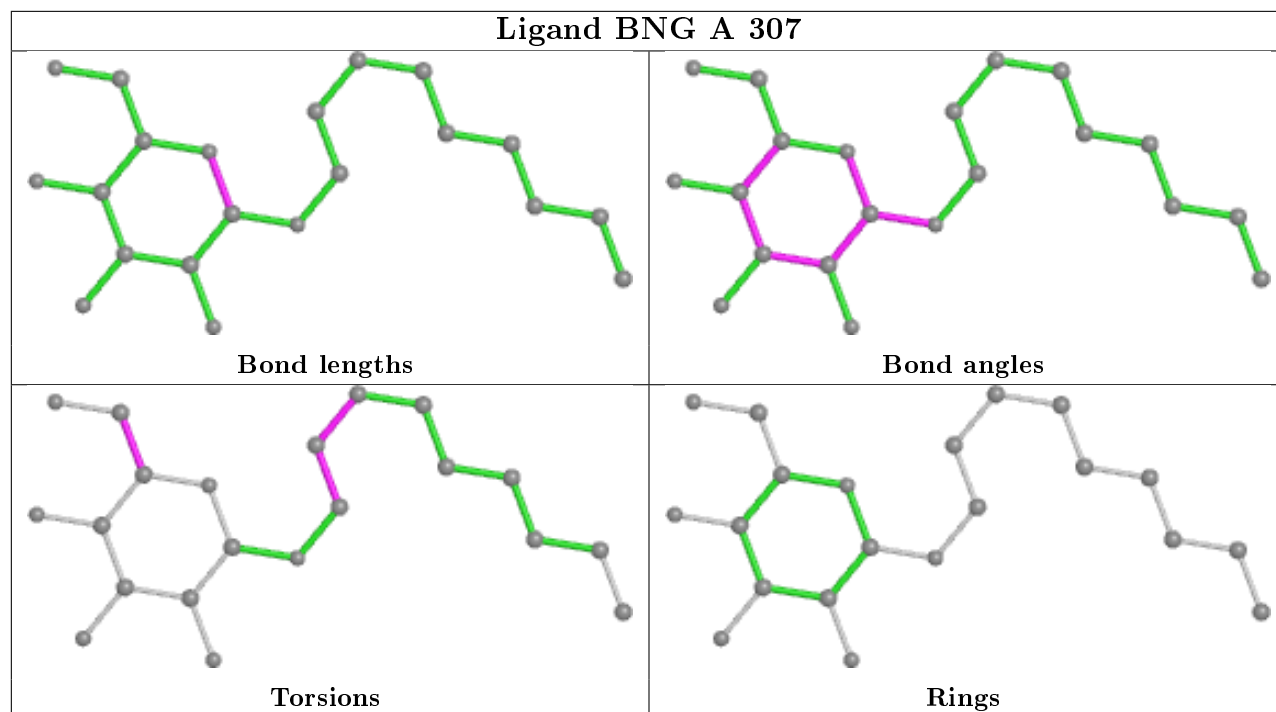
Mol	Chain	Res	Type	Atoms
3	A	303	PG4	C3-C4-O3-C5
2	A	301	B12	C14-C13-C48-C49
3	A	304	PG4	O2-C3-C4-O3

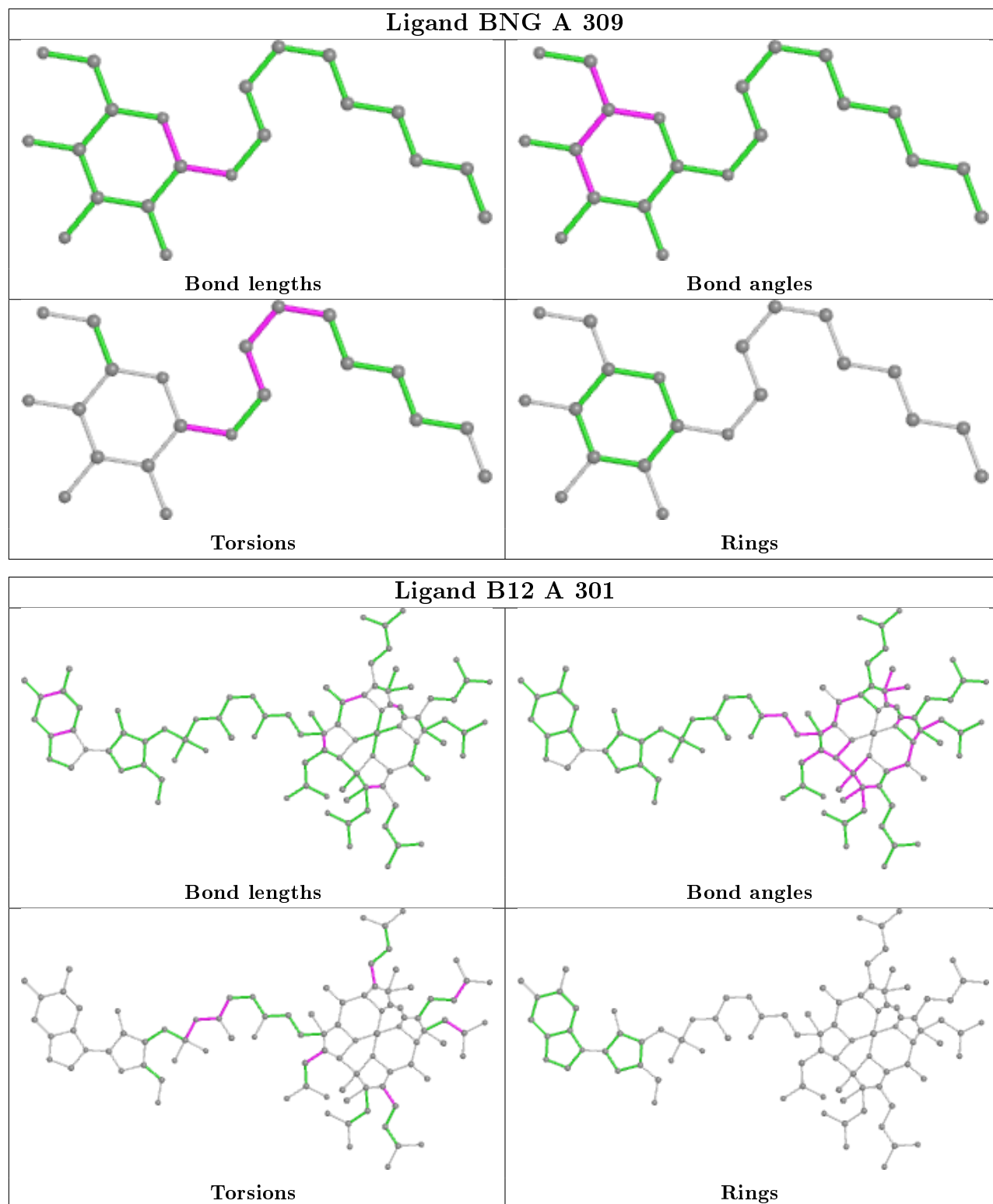
There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	PG4	1	0
4	A	307	BNG	1	0
3	A	305	PG4	1	0
4	A	308	BNG	1	0
4	A	309	BNG	3	0
2	A	301	B12	11	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	194/207 (93%)	1.18	46 (23%) 0 0	56, 72, 114, 183	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ALA	6.7
1	A	149	GLY	6.0
1	A	111	LEU	5.5
1	A	1	MET	5.3
1	A	73	TRP	5.2
1	A	199	ARG	5.1
1	A	114	PHE	5.0
1	A	200	HIS	4.8
1	A	117	ALA	4.6
1	A	86	TRP	4.5
1	A	109	SER	4.5
1	A	110	LEU	4.3
1	A	152	LEU	4.3
1	A	185	ARG	4.0
1	A	184	ARG	3.9
1	A	151	VAL	3.9
1	A	112	GLY	3.6
1	A	175	VAL	3.3
1	A	46	LEU	3.1
1	A	72	THR	3.1
1	A	13	ILE	3.1
1	A	121	LEU	3.0
1	A	155	GLU	3.0
1	A	146	THR	2.9
1	A	108	LEU	2.9
1	A	68	TYR	2.8
1	A	22	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.8
1	A	35	LEU	2.8
1	A	129	LEU	2.6
1	A	169	VAL	2.6
1	A	59	LEU	2.6
1	A	173	ALA	2.6
1	A	27[A]	HIS	2.5
1	A	147[A]	LEU	2.4
1	A	125	ALA	2.4
1	A	167	LEU	2.4
1	A	74	GLY	2.4
1	A	113	LEU	2.3
1	A	20	MET	2.3
1	A	181	ALA	2.2
1	A	170	GLY	2.2
1	A	17	LEU	2.2
1	A	171	LEU	2.1
1	A	118	GLY	2.0
1	A	144	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

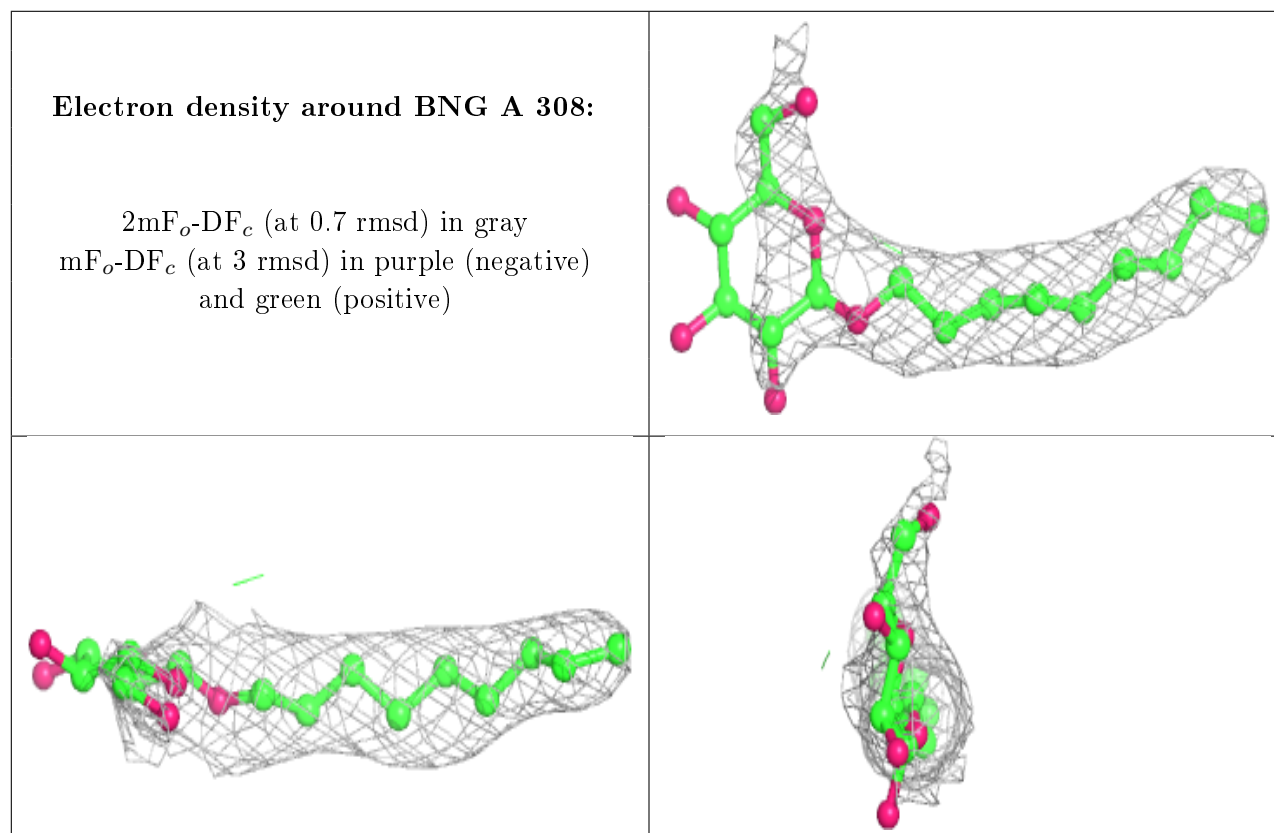
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	316	7/7	-0.03	0.33	146,147,148,149	0
3	PG4	A	306	13/13	0.14	0.34	136,148,153,156	0
6	PGE	A	317	10/10	0.33	0.28	108,133,136,142	0
4	BNG	A	308	21/21	0.40	0.43	79,129,159,168	0

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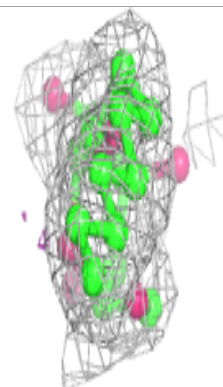
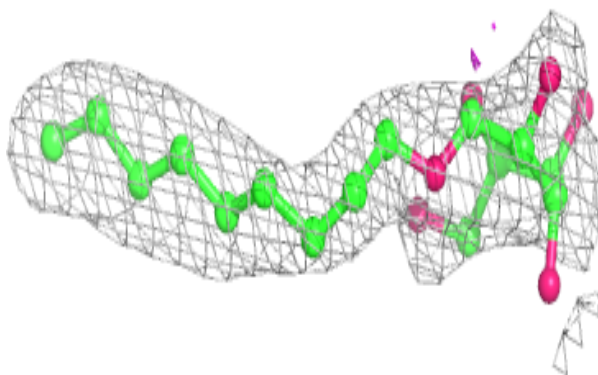
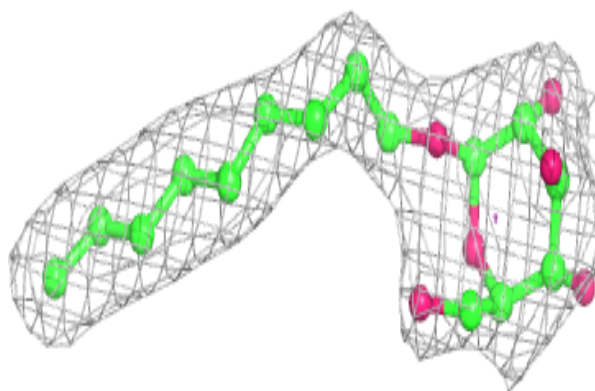
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	315	7/7	0.45	0.34	119,129,138,139	0
4	BNG	A	307	21/21	0.51	0.30	68,94,134,140	0
3	PG4	A	304	13/13	0.60	0.24	86,95,116,117	0
5	PEG	A	314	7/7	0.61	0.21	108,111,122,126	0
5	PEG	A	311	7/7	0.67	0.20	98,114,121,122	0
5	PEG	A	310	7/7	0.70	0.23	87,98,106,106	0
3	PG4	A	305	13/13	0.72	0.22	95,106,117,121	0
4	BNG	A	309	21/21	0.73	0.24	73,92,127,140	0
3	PG4	A	302	13/13	0.74	0.56	111,118,125,127	13
3	PG4	A	303	13/13	0.77	0.24	76,89,117,122	0
5	PEG	A	312	7/7	0.79	0.17	79,86,91,95	0
5	PEG	A	313	7/7	0.84	0.21	105,115,121,121	0
2	B12	A	301	91/91	0.89	0.14	49,64,80,101	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.

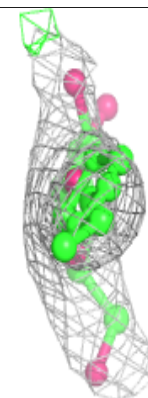
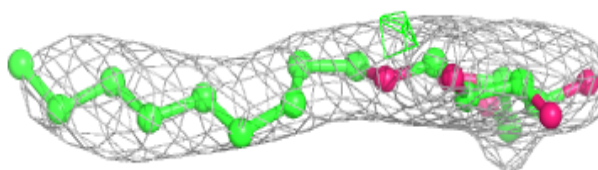
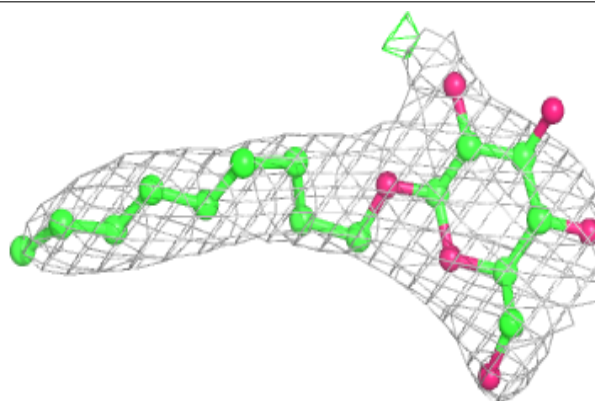


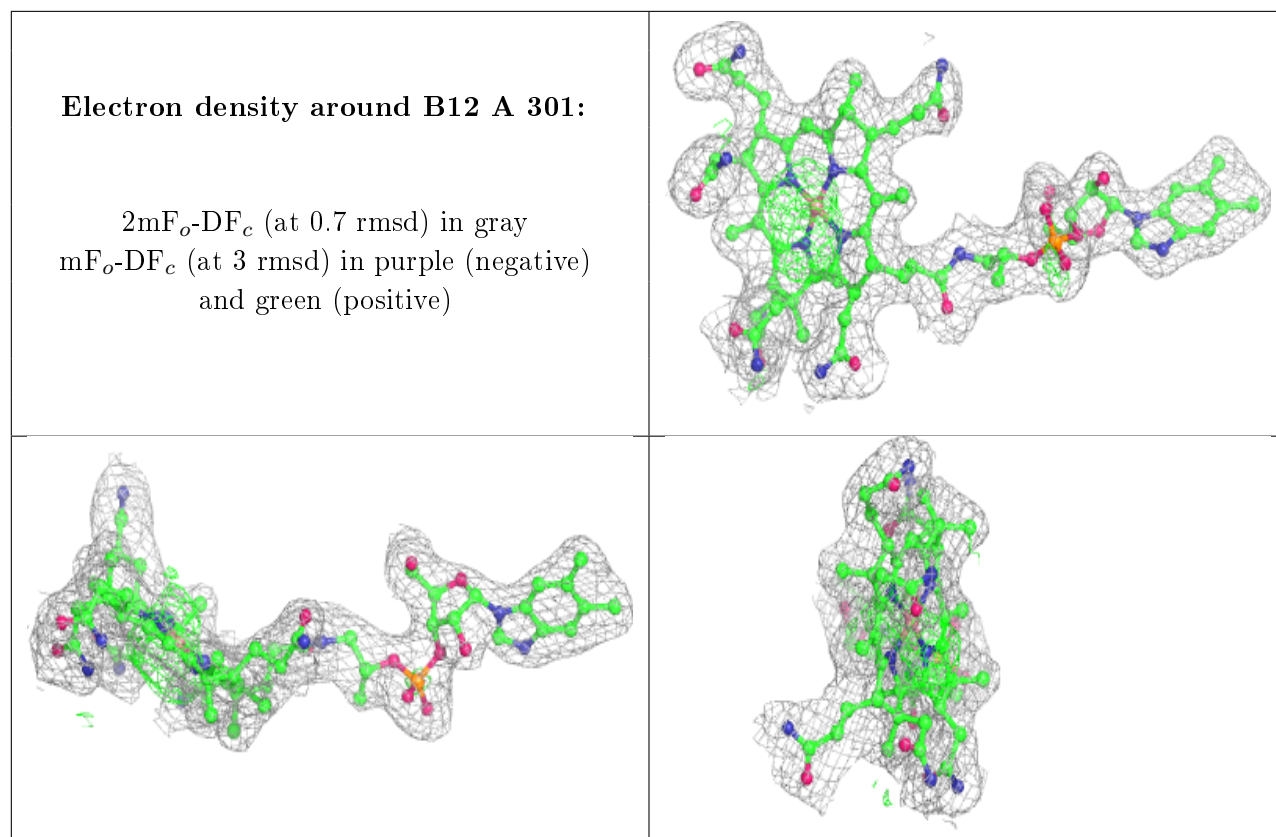
Electron density around BNG A 307:

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

**Electron density around BNG A 309:**

$2mF_o-DF_c$ (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.