wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 01:24 AM EDT

PDB ID	:	3NE2
Title	:	Archaeoglobus fulgidus aquaporin
Authors	:	Lee, J.K.; Finer-Moore, J.S.; Stroud, R.M.; Center for Structures of Membrane Proteins (CSMP)
Deposited on	:	2010-06-08
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

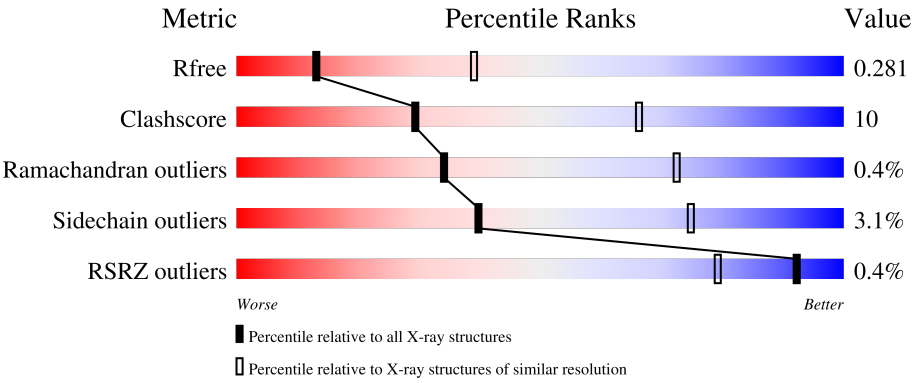
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 >=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 <=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	246	78% 21%
1	B	246	79% 20%
1	C	246	80% 20%
1	D	246	% 81% 18%
1	E	246	80% 20%

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Mol	Chain	Length	Quality of chain
1	F	246	
1	G	246	
1	H	246	

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	BOG	H	249	-	-	X	-

2 Entry composition (i)

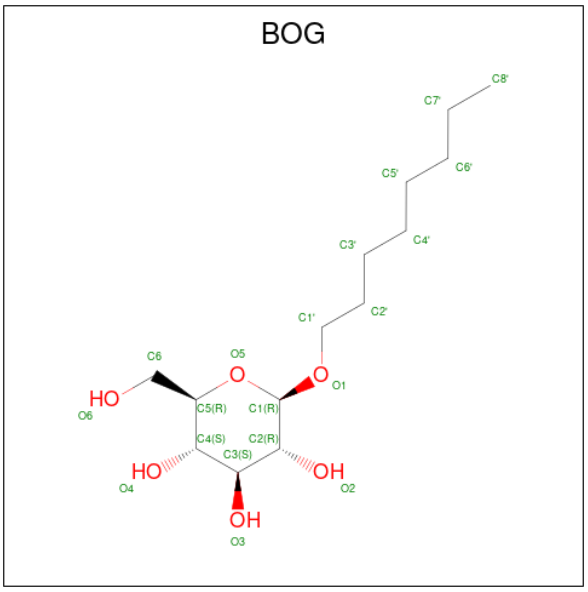
There are 3 unique types of molecules in this entry. The entry contains 14238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable aquaporin AqpM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1758	1169	279	303	7			
1	B	244	Total	C	N	O	S	0	0	0
			1760	1169	281	303	7			
1	C	246	Total	C	N	O	S	0	0	0
			1769	1174	282	305	8			
1	D	244	Total	C	N	O	S	0	0	0
			1746	1161	277	301	7			
1	E	245	Total	C	N	O	S	0	0	0
			1758	1169	279	302	8			
1	F	244	Total	C	N	O	S	0	0	0
			1748	1163	275	303	7			
1	G	244	Total	C	N	O	S	0	0	0
			1734	1155	271	301	7			
1	H	244	Total	C	N	O	S	0	0	0
			1756	1167	281	301	7			

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 14 6	0	0
2	A	1	Total C O 20 14 6	0	0
2	A	1	Total C O 20 14 6	0	0
2	D	1	Total C O 20 14 6	0	0
2	D	1	Total C O 20 14 6	0	0
2	F	1	Total C O 20 14 6	0	0
2	H	1	Total C O 20 14 6	0	0
2	H	1	Total C O 20 14 6	0	0
2	H	1	Total C O 20 14 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	4	Total O 4 4	0	0
3	C	4	Total O 4 4	0	0

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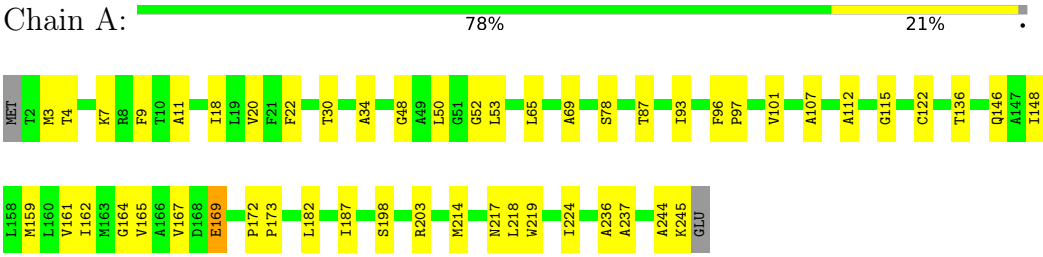
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total O 3 3	0	0
3	E	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	G	3	Total O 3 3	0	0
3	H	2	Total O 2 2	0	0

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.

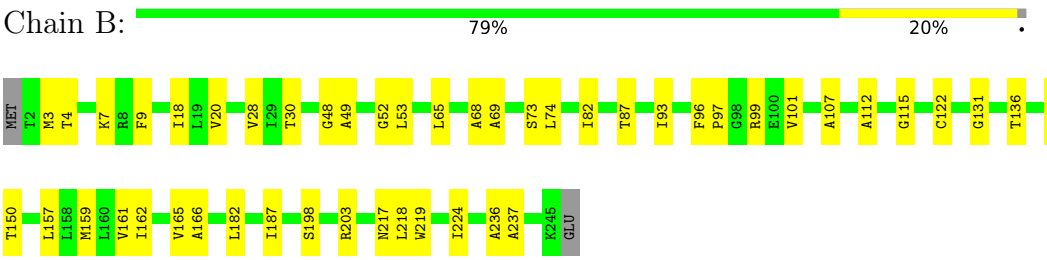
• Molecule 1: Probable aquaporin AqpM

Chain A:



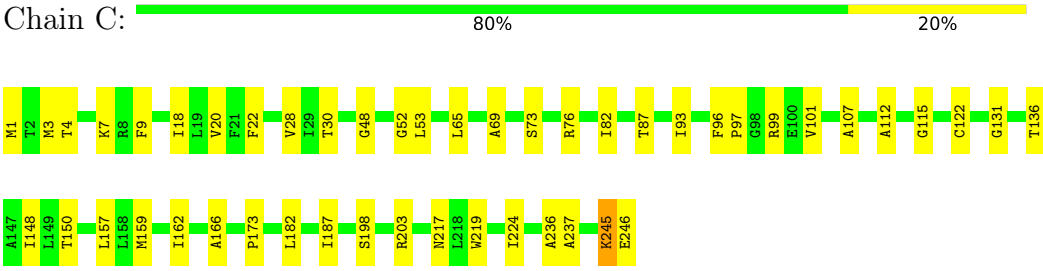
• Molecule 1: Probable aquaporin AqpM

Chain B:



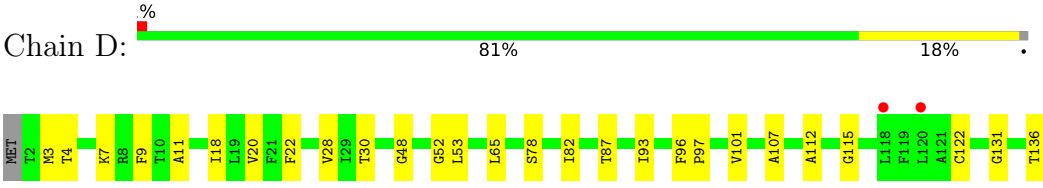
• Molecule 1: Probable aquaporin AqpM

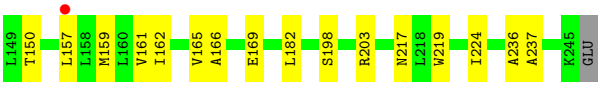
Chain C:



• Molecule 1: Probable aquaporin AqpM

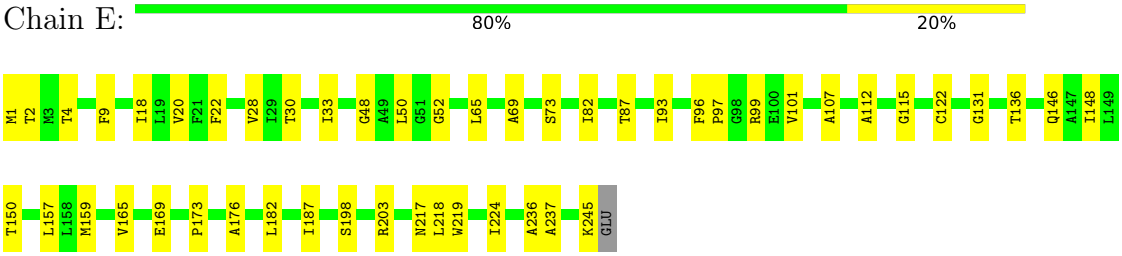
Chain D:





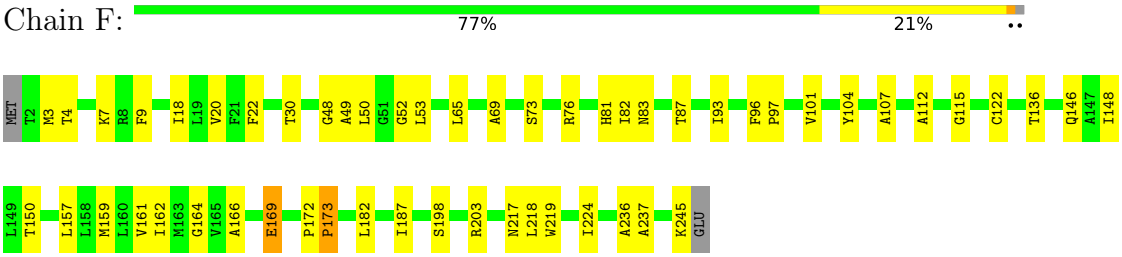
• Molecule 1: Probable aquaporin AqpM

Chain E:



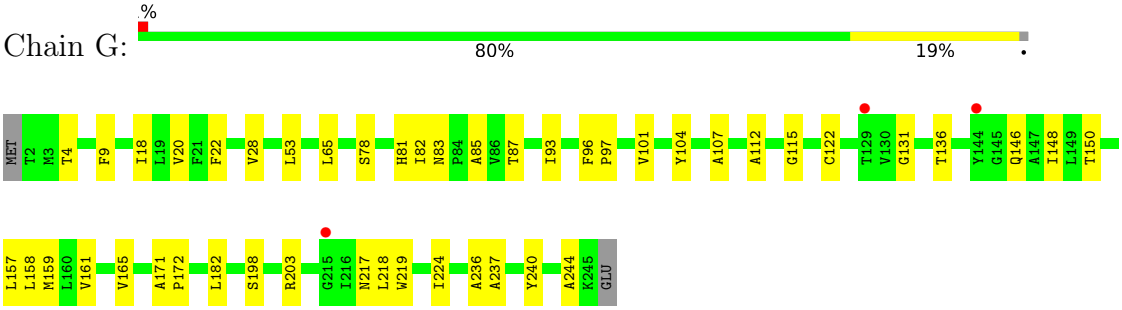
• Molecule 1: Probable aquaporin AqpM

Chain F:



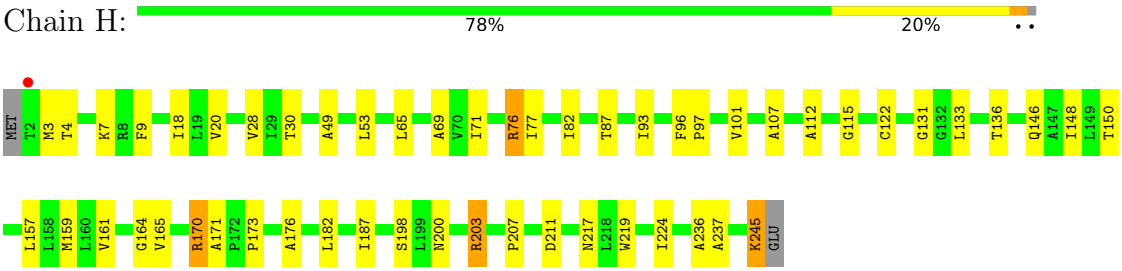
• Molecule 1: Probable aquaporin AqpM

Chain G:



• Molecule 1: Probable aquaporin AqpM

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.90Å 199.86Å 90.57Å 90.00° 117.51° 90.00°	Depositor
Resolution (Å)	39.07 – 3.00 39.07 – 3.00	Depositor EDS
% Data completeness (in resolution range)	61.8 (39.07-3.00) 61.8 (39.07-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 3.01Å)	Xtriage
Refinement program	REFMAC, ELVES	Depositor
R, R_{free}	0.245 , 0.274 0.253 , 0.281	Depositor DCC
R_{free} test set	1693 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	108.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 87.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14238	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BOG

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	0.72	0/1803	0.66	0/2467
1	B	0.52	0/1805	0.59	0/2470
1	C	0.61	0/1814	0.65	1/2483 (0.0%)
1	D	0.47	0/1791	0.54	0/2454
1	E	0.52	0/1803	0.59	0/2468
1	F	0.74	1/1793 (0.1%)	0.65	0/2456
1	G	0.45	0/1779	0.53	0/2440
1	H	0.52	0/1801	0.58	0/2465
All	All	0.58	1/14389 (0.0%)	0.60	1/19703 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	169	GLU	CG-CD	6.38	1.61	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	245	LYS	N-CA-C	7.67	131.70	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	MET	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	1758	0	1808	51	0
1	B	1760	0	1808	39	0
1	C	1769	0	1811	42	0
1	D	1746	0	1782	33	0
1	E	1758	0	1805	39	0
1	F	1748	0	1786	50	0
1	G	1734	0	1760	34	0
1	H	1756	0	1804	57	0
2	A	60	0	84	1	0
2	D	40	0	56	1	0
2	F	20	0	28	0	0
2	H	60	0	84	11	0
3	A	8	0	0	1	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	3	0	0	0	0
3	E	2	0	0	2	0
3	F	3	0	0	0	0
3	G	3	0	0	3	0
3	H	2	0	0	3	0
All	All	14238	0	14616	274	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 10.

The worst 5 of 274 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:C:93:ILE:HD11	1:C:237:ALA:HB1	1.25	1.16
1:F:93:ILE:HD11	1:F:237:ALA:HB1	1.17	1.13
1:E:93:ILE:HD11	1:E:237:ALA:HB1	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HD11	1:D:237:ALA:HB1	1.30	1.07
1:A:93:ILE:HD11	1:A:237:ALA:HB1	1.34	1.07

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	242/246 (98%)	227 (94%)	15 (6%)	0	100	100
1	B	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	34	72
1	C	244/246 (99%)	230 (94%)	13 (5%)	1 (0%)	34	72
1	D	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	34	72
1	E	243/246 (99%)	229 (94%)	13 (5%)	1 (0%)	34	72
1	F	242/246 (98%)	227 (94%)	14 (6%)	1 (0%)	34	72
1	G	242/246 (98%)	228 (94%)	13 (5%)	1 (0%)	34	72
1	H	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	34	72
All	All	1939/1968 (98%)	1832 (94%)	100 (5%)	7 (0%)	34	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	82	ILE
1	B	82	ILE
1	E	82	ILE
1	G	82	ILE
1	H	82	ILE

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	170/173 (98%)	164 (96%)	6 (4%)	36	71
1	B	170/173 (98%)	166 (98%)	4 (2%)	49	79
1	C	170/173 (98%)	166 (98%)	4 (2%)	49	79
1	D	167/173 (96%)	164 (98%)	3 (2%)	59	85
1	E	169/173 (98%)	161 (95%)	8 (5%)	26	63
1	F	168/173 (97%)	161 (96%)	7 (4%)	30	66
1	G	165/173 (95%)	161 (98%)	4 (2%)	49	79
1	H	169/173 (98%)	163 (96%)	6 (4%)	35	70
All	All	1348/1384 (97%)	1306 (97%)	42 (3%)	40	75

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	173	PRO
1	G	218	LEU
1	F	203	ARG
1	G	4	THR
1	H	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	241	ASN
1	G	241	ASN
1	E	241	ASN
1	D	241	ASN
1	F	241	ASN

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)

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	BOG	H	247	-	20,20,20	0.86	1 (5%)	25,25,25	1.84	6 (24%)
2	BOG	D	247	-	20,20,20	0.69	1 (5%)	25,25,25	1.42	6 (24%)
2	BOG	A	247	-	20,20,20	0.65	1 (5%)	25,25,25	1.06	1 (4%)
2	BOG	A	249	-	20,20,20	0.85	1 (5%)	25,25,25	1.21	3 (12%)
2	BOG	F	247	-	20,20,20	0.68	1 (5%)	25,25,25	0.65	0
2	BOG	H	249	-	20,20,20	0.72	1 (5%)	25,25,25	1.28	3 (12%)
2	BOG	H	248	-	20,20,20	0.77	1 (5%)	25,25,25	0.91	1 (4%)
2	BOG	D	248	-	20,20,20	0.74	1 (5%)	25,25,25	1.45	3 (12%)
2	BOG	A	248	-	20,20,20	0.85	1 (5%)	25,25,25	1.34	5 (20%)

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	BOG	H	247	-	-	10/11/31/31	0/1/1/1
2	BOG	D	247	-	-	7/11/31/31	0/1/1/1
2	BOG	A	247	-	-	6/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	A	249	-	-	6/11/31/31	0/1/1/1
2	BOG	F	247	-	-	6/11/31/31	0/1/1/1
2	BOG	H	249	-	-	8/11/31/31	0/1/1/1
2	BOG	H	248	-	-	6/11/31/31	0/1/1/1
2	BOG	D	248	-	-	7/11/31/31	0/1/1/1
2	BOG	A	248	-	-	6/11/31/31	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249	BOG	O1-C1	3.10	1.45	1.40
2	H	247	BOG	O1-C1	2.92	1.45	1.40
2	H	248	BOG	O1-C1	2.72	1.44	1.40
2	A	248	BOG	O1-C1	2.68	1.44	1.40
2	F	247	BOG	O1-C1	2.39	1.44	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	247	BOG	C1-O5-C5	5.04	123.57	113.69
2	D	248	BOG	O1-C1-C2	4.47	115.29	108.30
2	H	249	BOG	C4-C3-C2	4.12	118.02	110.82
2	H	247	BOG	C3-C4-C5	3.57	116.61	110.24
2	A	247	BOG	O1-C1-C2	3.52	113.79	108.30

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	249	BOG	C2-C1-O1-C1'
2	A	249	BOG	O5-C1-O1-C1'
2	F	247	BOG	C2-C1-O1-C1'
2	F	247	BOG	O5-C1-O1-C1'
2	H	247	BOG	C2-C1-O1-C1'

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	247	BOG	1	0

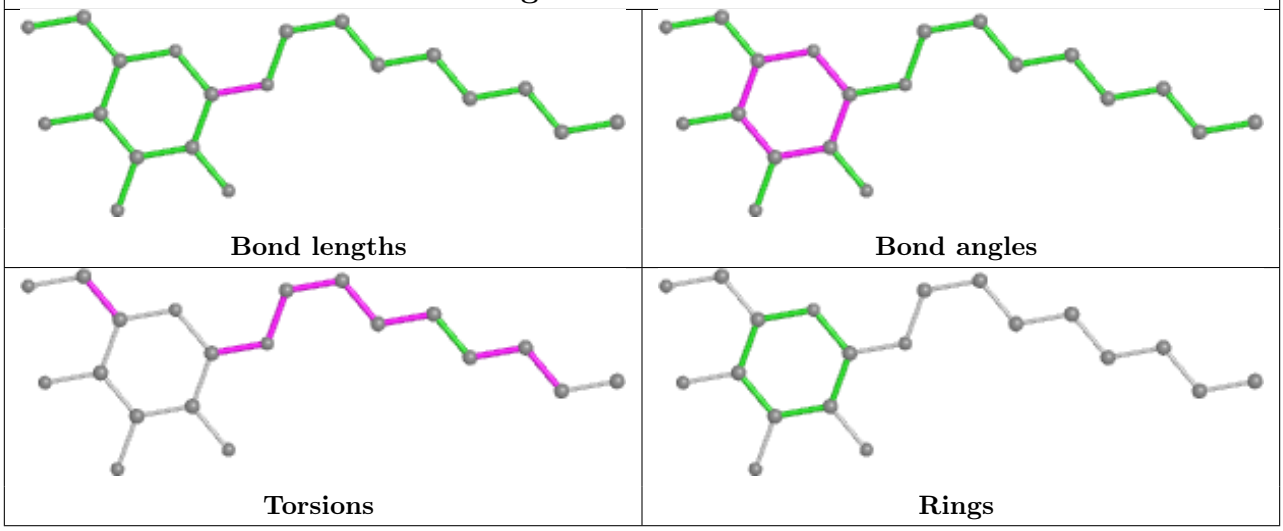
Continued on next page...

Continued from previous page...

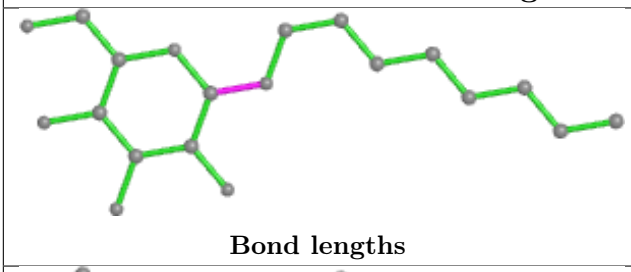
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	249	BOG	11	0
2	D	248	BOG	1	0
2	A	248	BOG	1	0

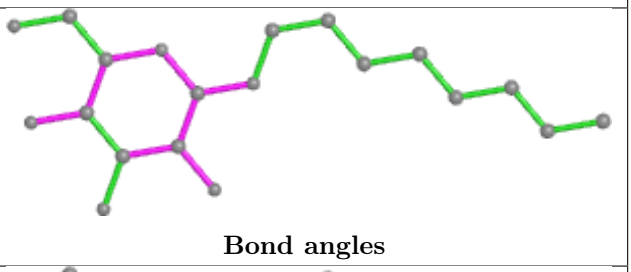
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

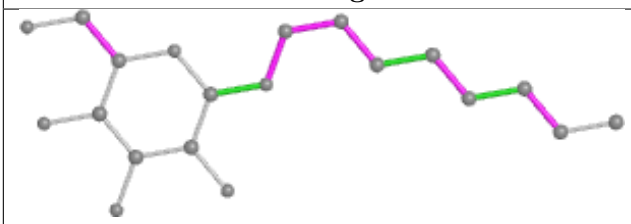
Ligand BOG H 247

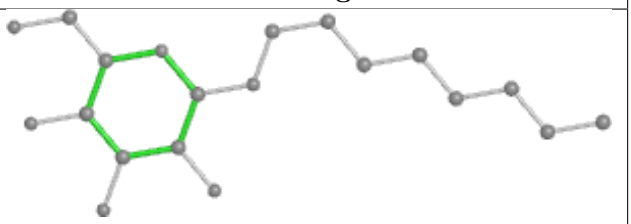


Ligand BOG D 247

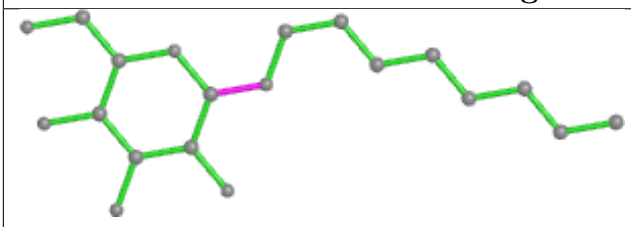

Bond lengths

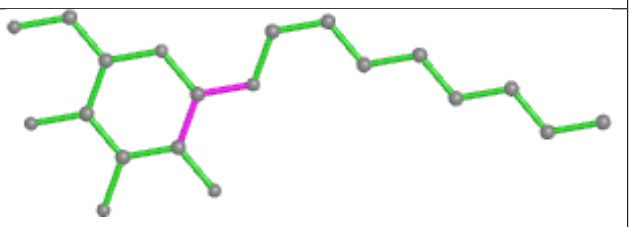

Bond angles

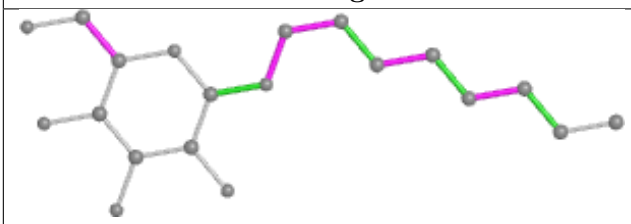

Torsions

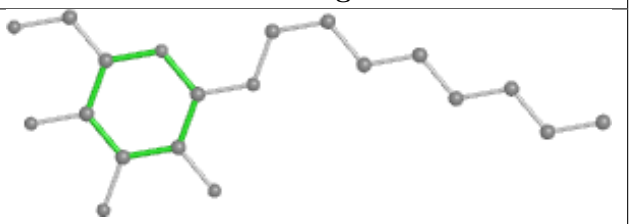

Rings

Ligand BOG A 247

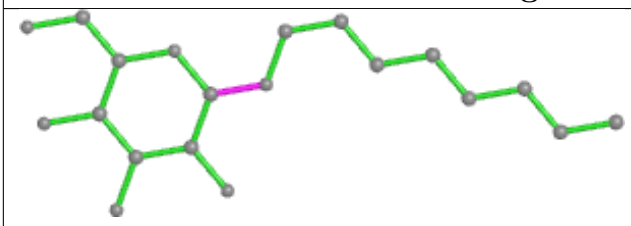

Bond lengths

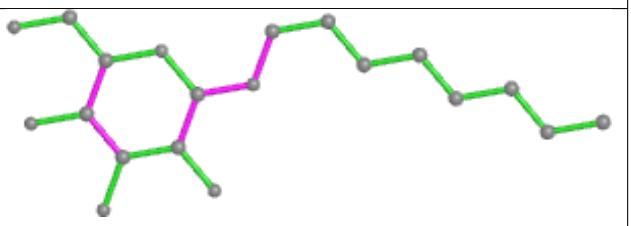

Bond angles

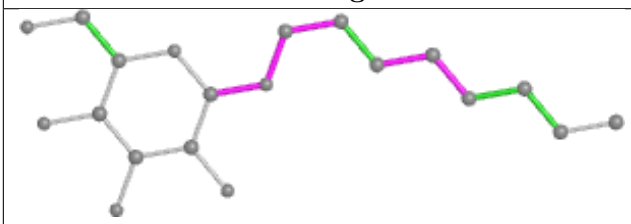

Torsions

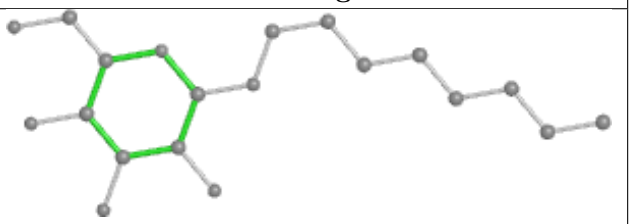

Rings

Ligand BOG A 249

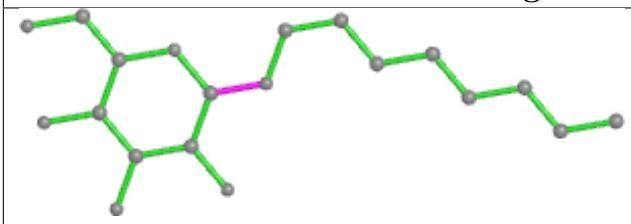

Bond lengths


Bond angles

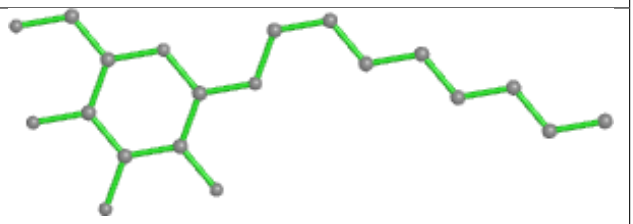

Torsions


Rings

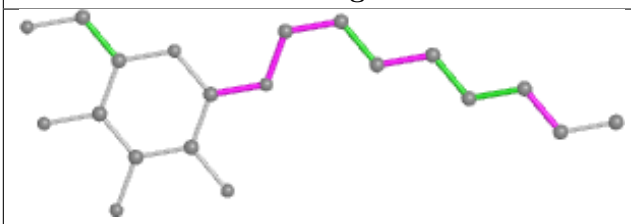
Ligand BOG F 247



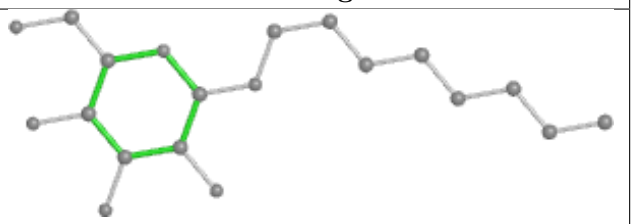
Bond lengths



Bond angles

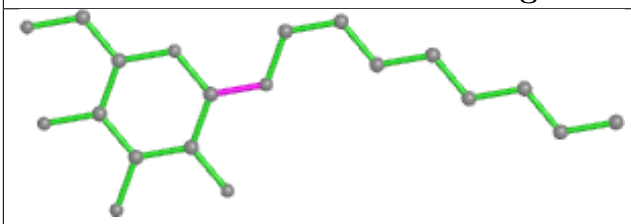


Torsions

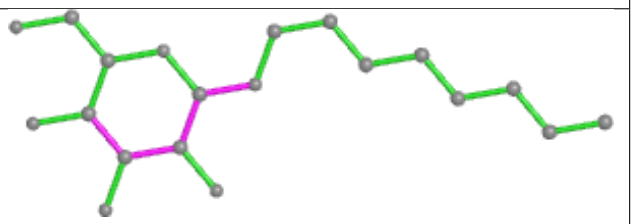


Rings

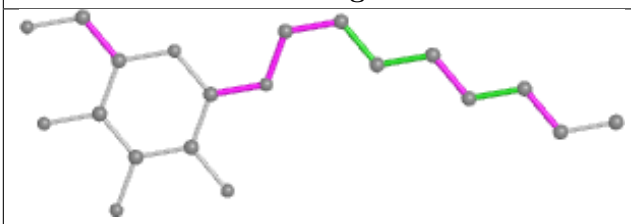
Ligand BOG H 249



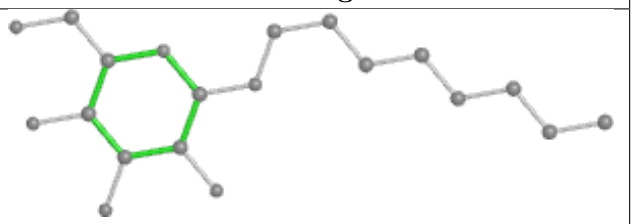
Bond lengths



Bond angles

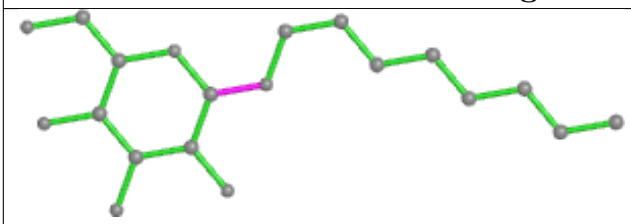


Torsions

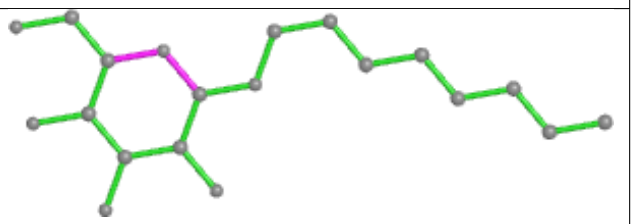


Rings

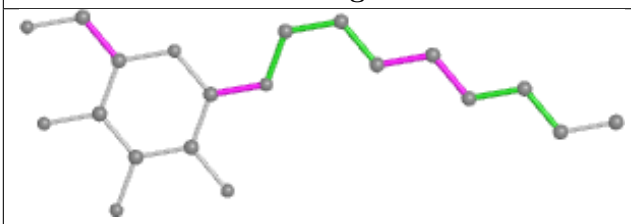
Ligand BOG H 248



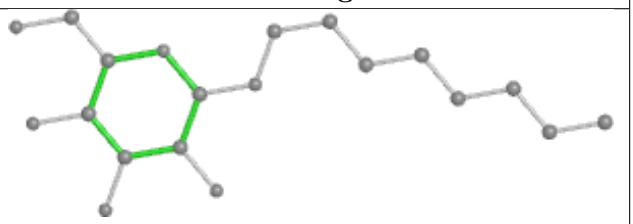
Bond lengths



Bond angles

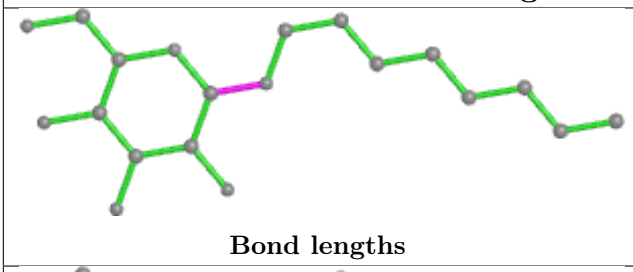


Torsions

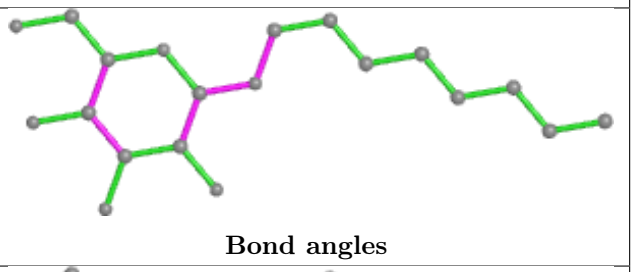


Rings

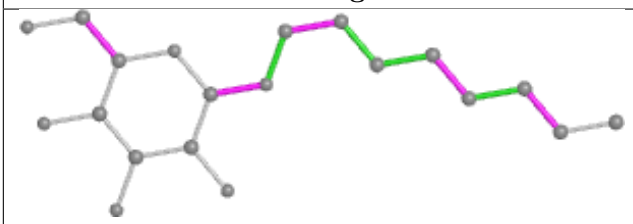
Ligand BOG D 248



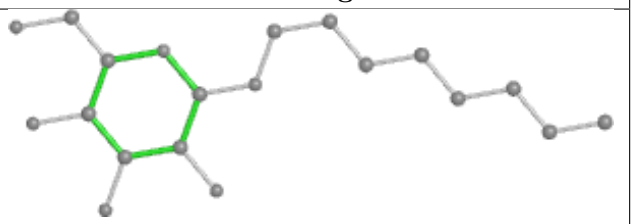
Bond lengths



Bond angles

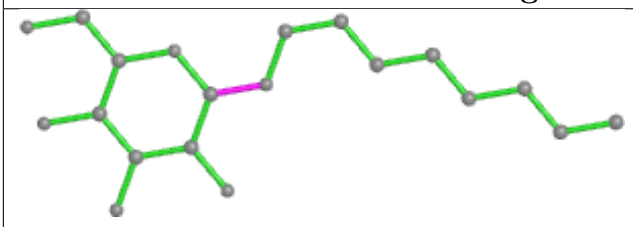


Torsions

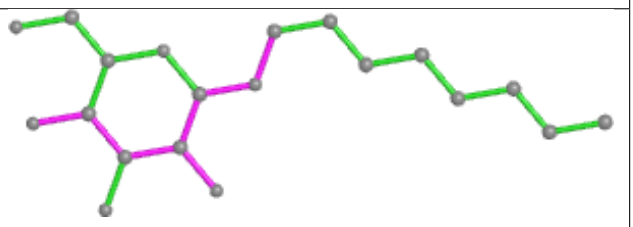


Rings

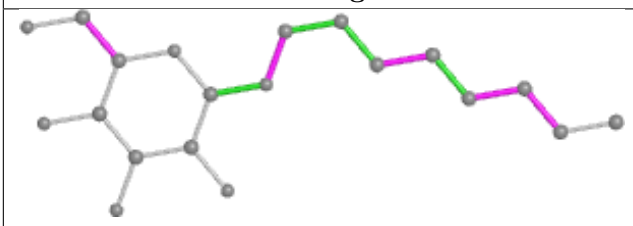
Ligand BOG A 248



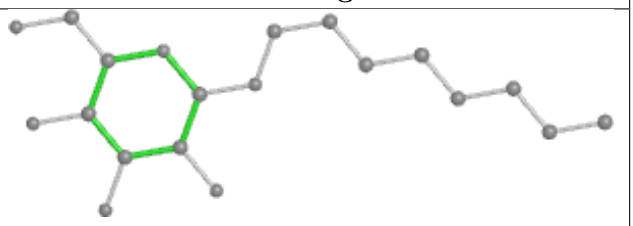
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	244/246 (99%)	-0.46	0 100 100	74, 98, 127, 141	0
1	B	244/246 (99%)	-0.28	0 100 100	91, 137, 194, 221	0
1	C	246/246 (100%)	-0.38	1 (0%) 92 79	79, 118, 178, 219	0
1	D	244/246 (99%)	-0.15	3 (1%) 79 54	115, 181, 231, 268	0
1	E	245/246 (99%)	-0.25	0 100 100	95, 149, 217, 262	0
1	F	244/246 (99%)	-0.47	0 100 100	75, 95, 123, 144	0
1	G	244/246 (99%)	-0.25	3 (1%) 79 54	122, 192, 253, 279	0
1	H	244/246 (99%)	-0.26	1 (0%) 92 79	97, 135, 192, 216	0
All	All	1955/1968 (99%)	-0.31	8 (0%) 92 79	74, 133, 218, 279	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	THR	8.4
1	G	144	TYR	4.5
1	D	120	LEU	3.3
1	G	129	THR	2.4
1	D	118	LEU	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

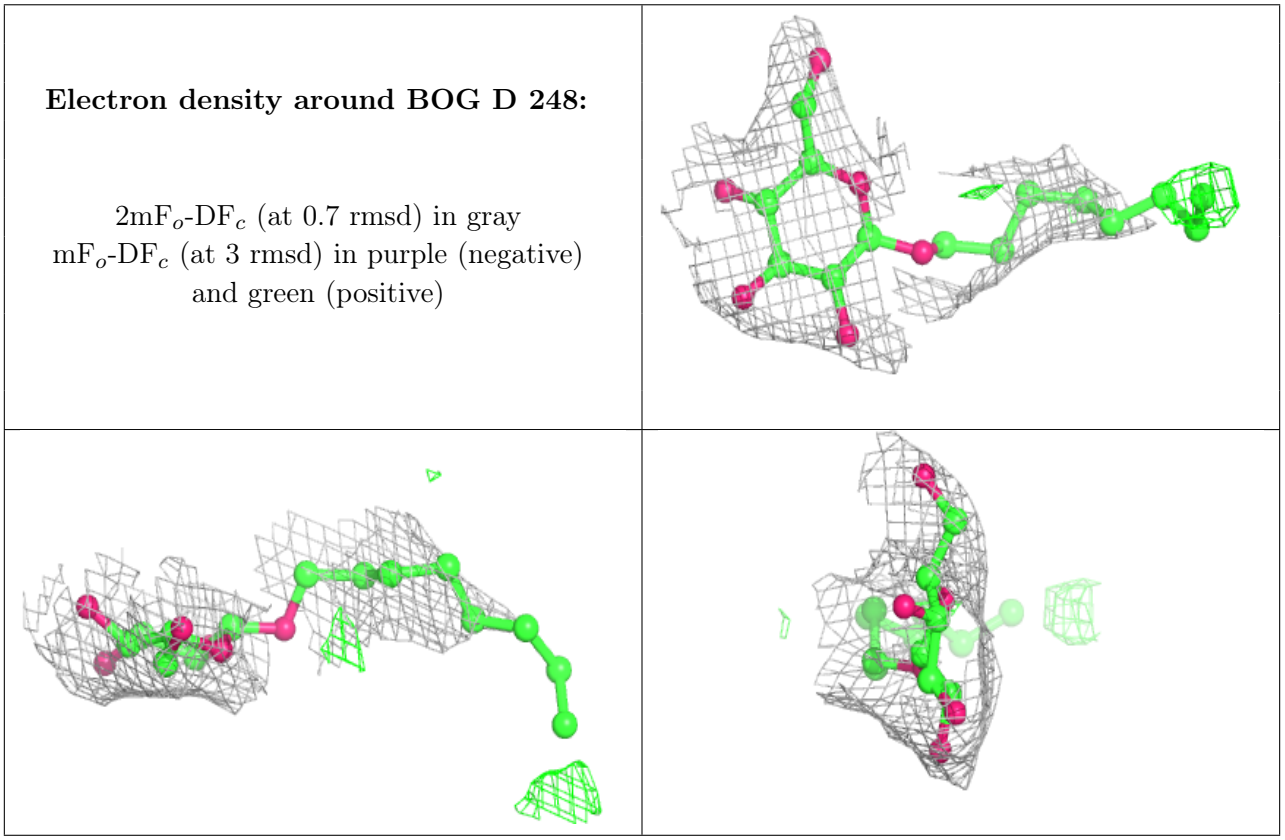
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BOG	D	248	20/20	0.83	0.19	171,173,174,174	0
2	BOG	A	248	20/20	0.85	0.14	140,146,148,148	0
2	BOG	H	249	20/20	0.85	0.17	188,190,191,191	0
2	BOG	A	247	20/20	0.87	0.21	151,154,156,157	0
2	BOG	H	248	20/20	0.89	0.13	172,180,181,182	0
2	BOG	A	249	20/20	0.90	0.16	160,166,166,167	0
2	BOG	D	247	20/20	0.91	0.23	181,183,184,184	0
2	BOG	F	247	20/20	0.93	0.20	133,135,140,140	0
2	BOG	H	247	20/20	0.94	0.20	112,118,121,122	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.

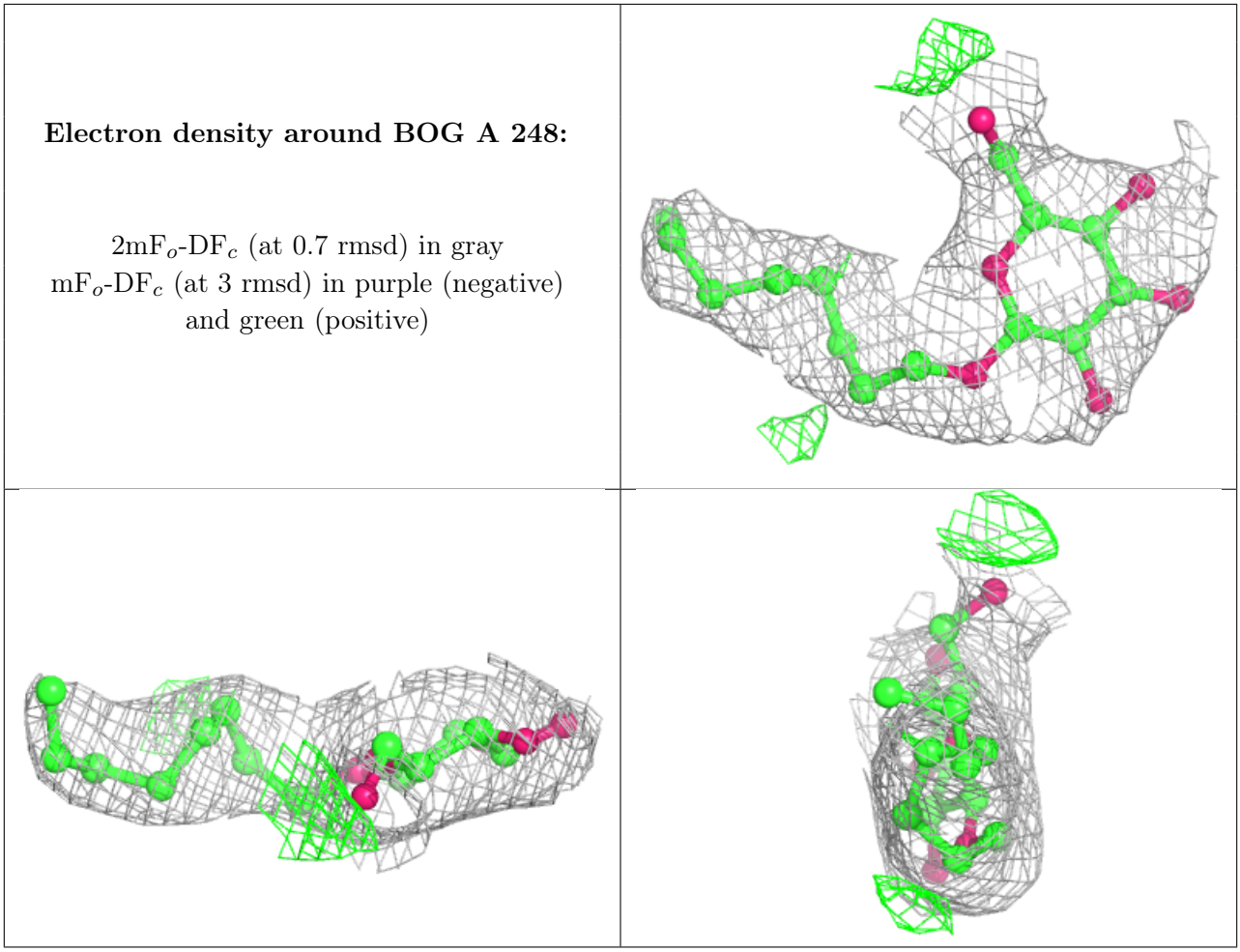
Electron density around BOG D 248:

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



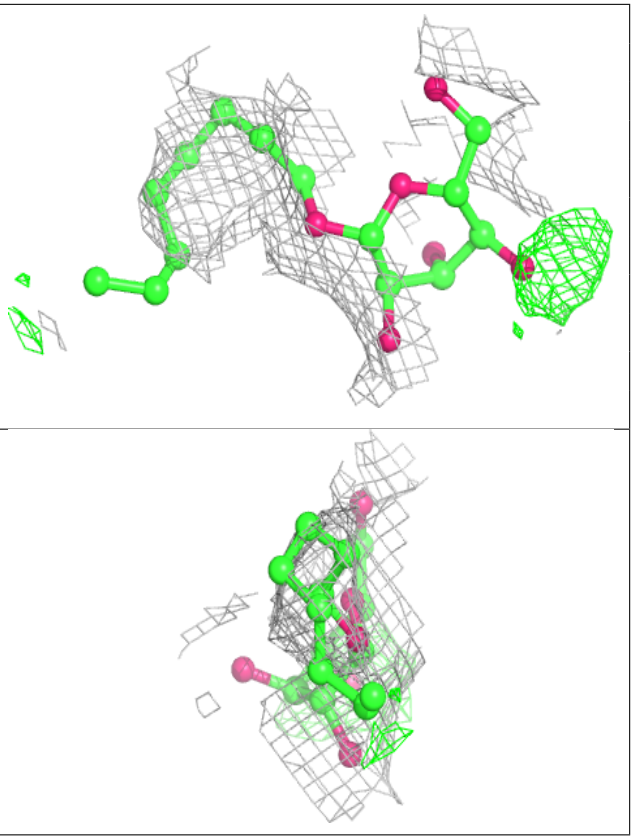
Electron density around BOG A 248:

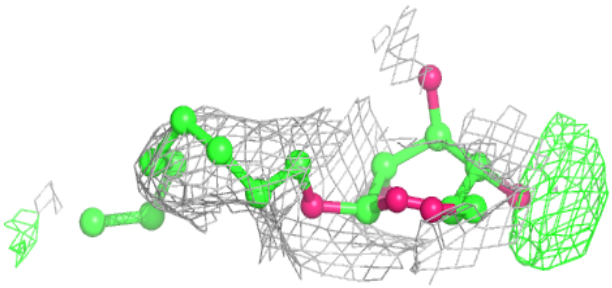
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BOG H 249:

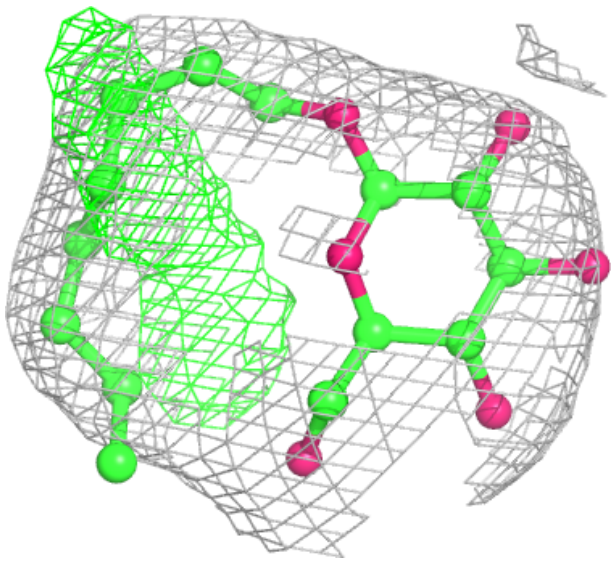
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

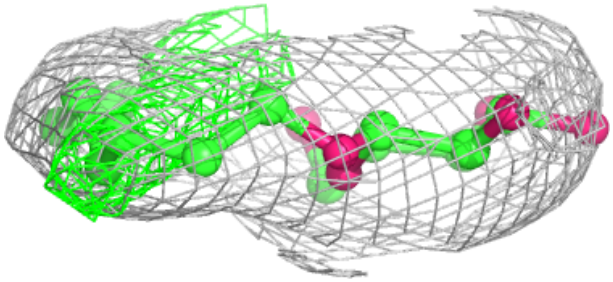


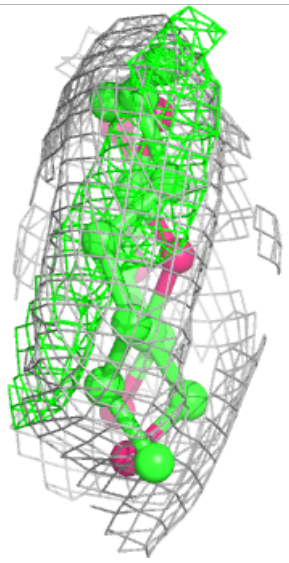


Electron density around BOG A 247:

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

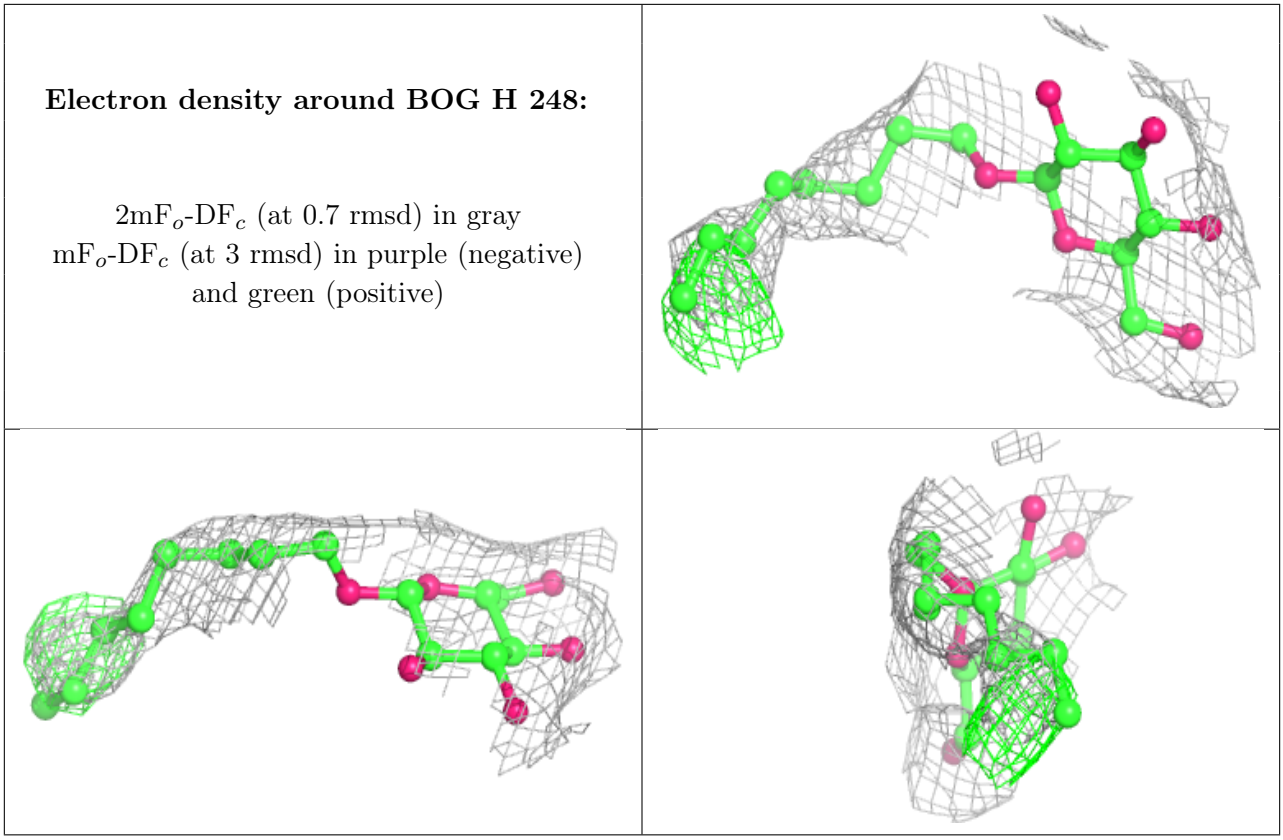






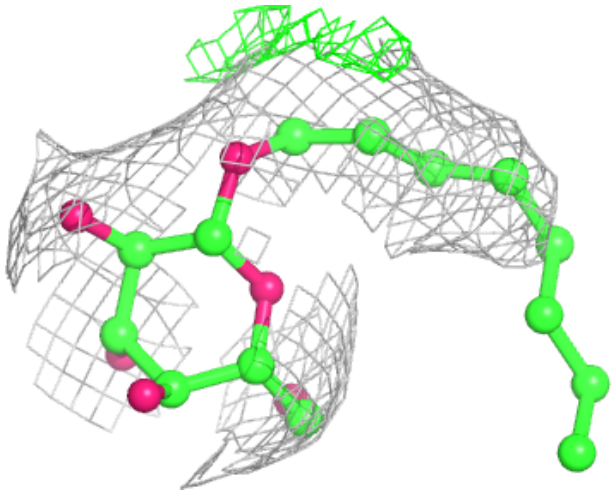
Electron density around BOG H 248:

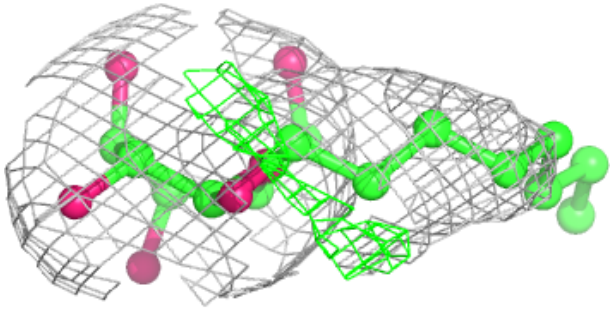
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

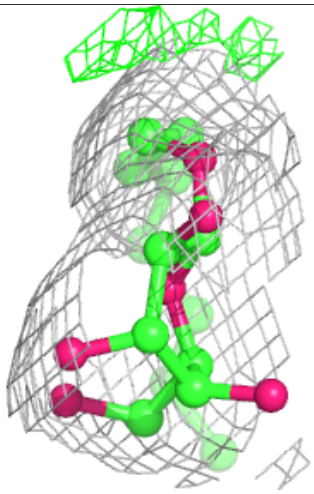


Electron density around BOG A 249:

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

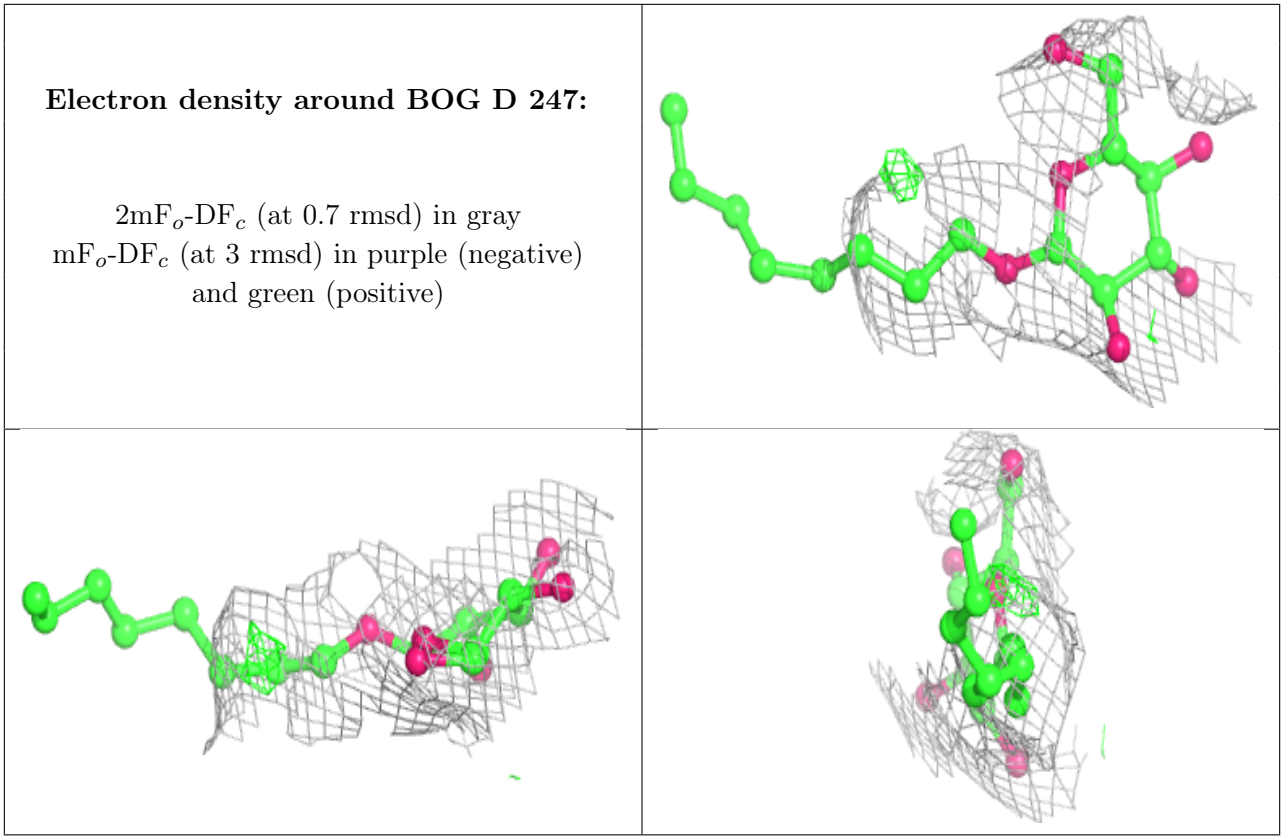






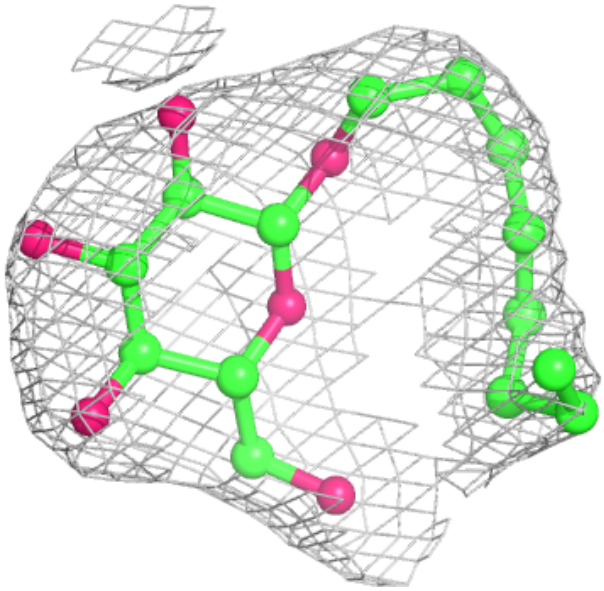
Electron density around BOG D 247:

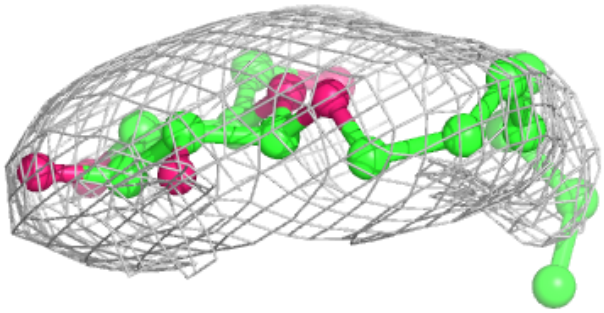
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

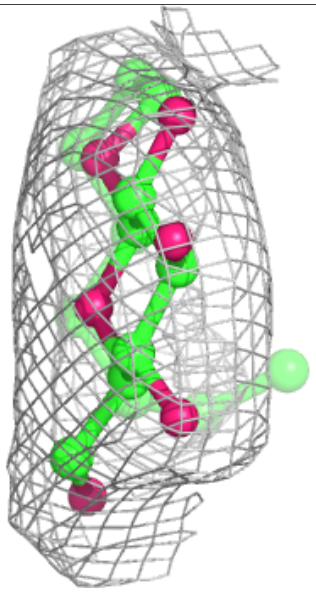


Electron density around BOG F 247:

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

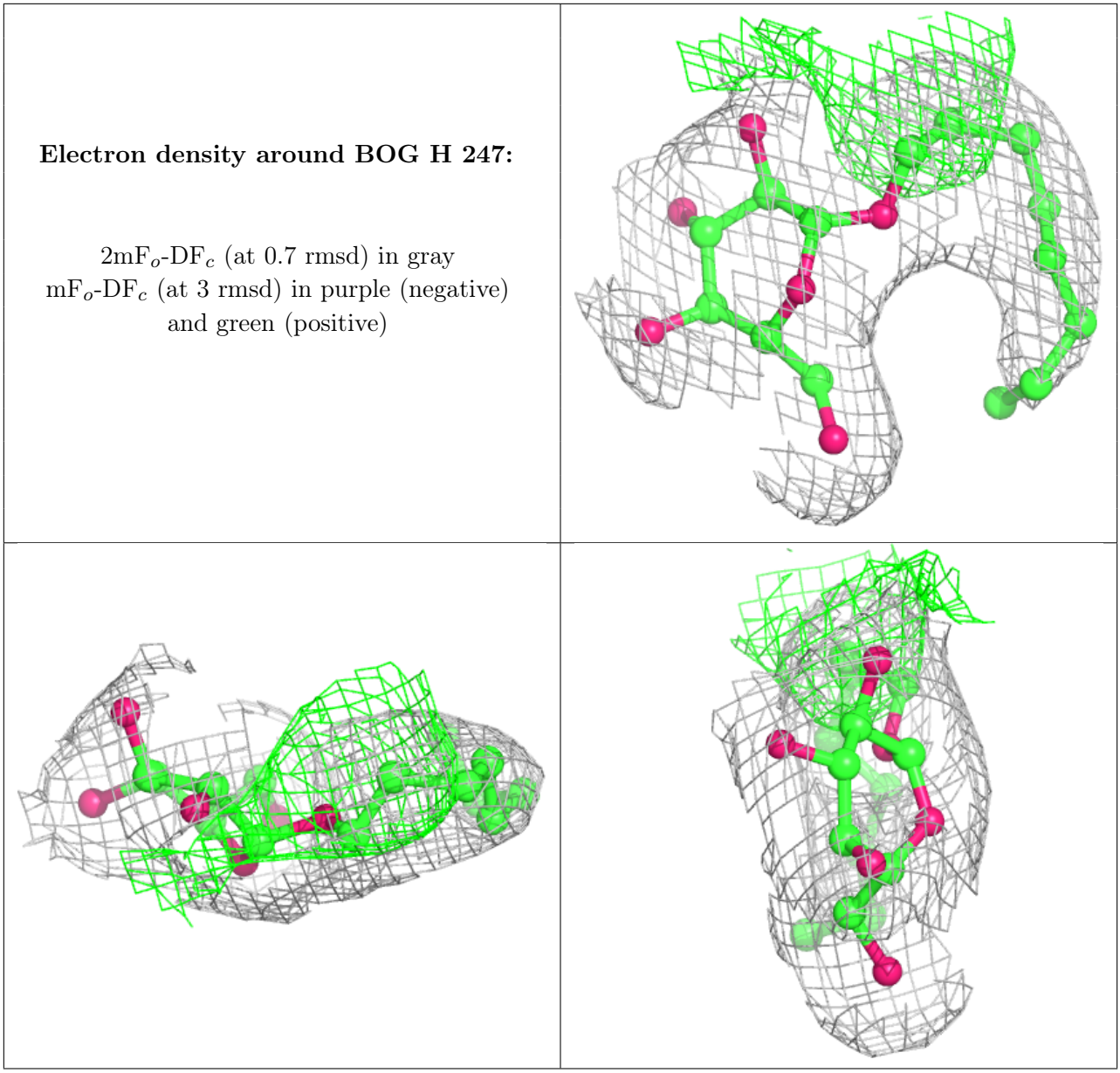






Electron density around BOG H 247:

$2mF_o$-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.