Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 08:07 AM EDT

PDB ID	:	6E4V
Title	:	The Crystal Structure of FhuE from E. coli in complex with its substrate Coprogen
Authors	:	Grinter, R.; Lithgow, T.
Deposited on	:	2018-07-18
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

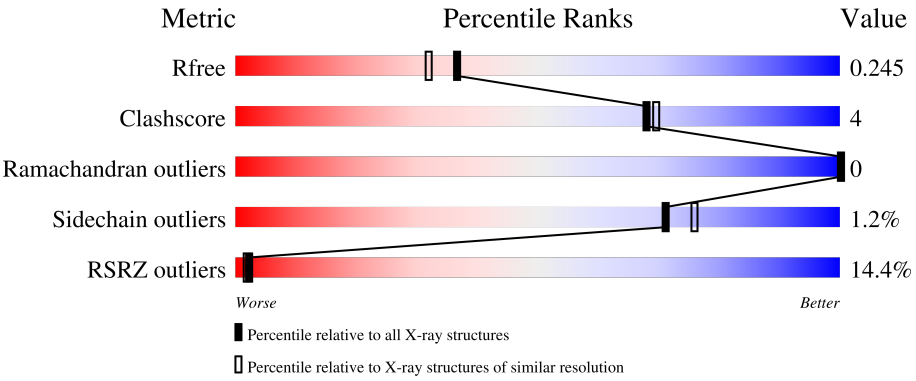
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	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 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	693	14% 90% 7%

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	HWS	A	806	X	-	-	-

2 Entry composition

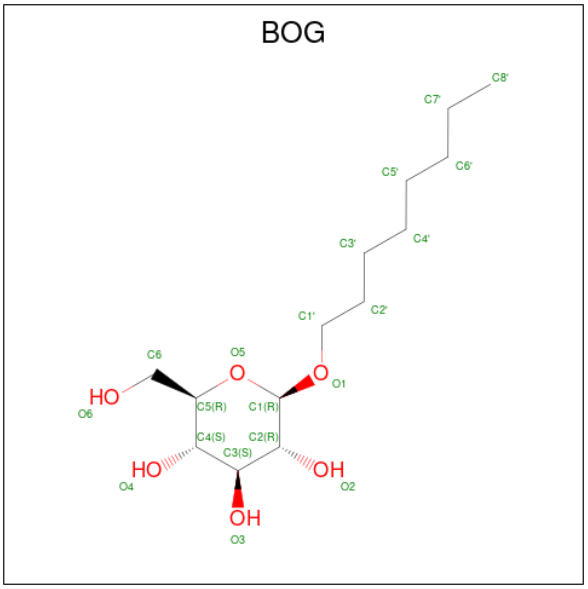
There are 4 unique types of molecules in this entry. The entry contains 5809 atoms, of which 140 are hydrogens and 0 are deuteriums.

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 FhuE receptor.

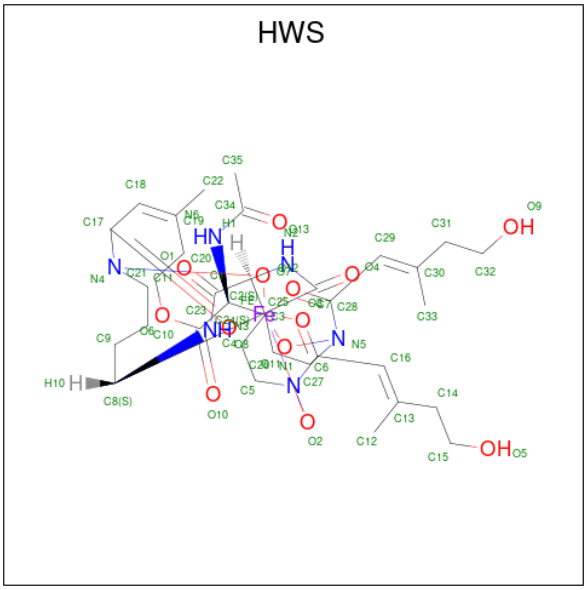
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5319	3335	903	1063	18			

- 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	H	O	0	0
			48	14	28	6		
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	A	1	Total	C	H	O	0	0
			48	14	28	6		
2	A	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 3 is COPROGEN (three-letter code: HWS) (formula: $C_{35}H_{53}FeN_6O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			54	34	1	6	13		

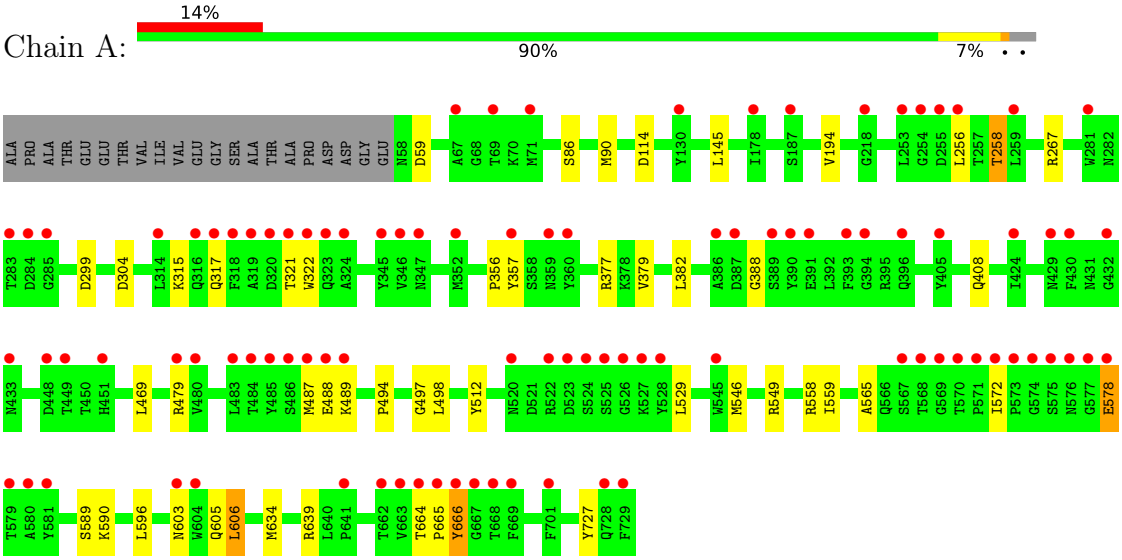
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		

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: FhuE receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.19Å 103.86Å 118.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.00 47.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	60.1 (47.57-2.00) 60.2 (47.57-2.00)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.11 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.206 , 0.235 0.226 , 0.245	Depositor DCC
R_{free} test set	1741 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5809	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: HWS, 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	0.63	0/5448	0.75	1/7409 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ASP	CB-CG-OD1	6.36	124.02	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5319	0	5002	40	0
2	A	100	140	140	2	0
3	A	54	0	0	0	0
4	A	196	0	0	0	0
All	All	5669	140	5142	40	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 4.

All (40) 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:A:664:THR:HB	1:A:665:PRO:HD2	1.47	0.93
1:A:258:THR:HG22	1:A:315:LYS:HB2	1.56	0.83
1:A:572:ILE:HD12	1:A:578:GLU:HB3	1.62	0.81
1:A:558:ARG:HD2	1:A:590:LYS:HE3	1.69	0.74
1:A:596:LEU:HD22	1:A:606:LEU:HD12	1.69	0.74
1:A:606:LEU:C	1:A:606:LEU:HD13	2.13	0.68
1:A:382:LEU:C	1:A:382:LEU:HD12	2.15	0.67
1:A:382:LEU:HD12	1:A:382:LEU:O	1.95	0.66
1:A:664:THR:CB	1:A:665:PRO:HD2	2.23	0.65
1:A:322:TRP:CD2	1:A:388:GLY:HA3	2.31	0.64
1:A:494:PRO:HG2	1:A:512:TYR:HE2	1.63	0.64
1:A:596:LEU:HD22	1:A:606:LEU:CD1	2.28	0.64
1:A:603:ASN:HB2	1:A:639:ARG:HB3	1.80	0.64
1:A:487:MET:HE3	1:A:489:LYS:HE3	1.80	0.63
1:A:256:LEU:HB3	1:A:317:GLN:HB3	1.83	0.60
1:A:546:MET:HB2	1:A:549:ARG:HB2	1.84	0.59
1:A:321:THR:O	1:A:388:GLY:HA2	2.03	0.57
1:A:559:ILE:HB	1:A:589:SER:OG	2.06	0.55
1:A:379:VAL:HG22	1:A:408:GLN:HG3	1.89	0.55
1:A:356:PRO:HG2	1:A:357:TYR:CE2	2.45	0.51
1:A:469:LEU:HD13	1:A:498:LEU:HD13	1.93	0.51
1:A:469:LEU:HD12	1:A:497:GLY:O	2.11	0.50
1:A:479:ARG:HG3	1:A:488:GLU:HG3	1.94	0.49
1:A:529:LEU:HD23	1:A:565:ALA:HB2	1.94	0.48
1:A:596:LEU:CD2	1:A:606:LEU:HD12	2.41	0.48
1:A:596:LEU:C	1:A:596:LEU:HD23	2.35	0.47
1:A:145:LEU:HD12	1:A:377:ARG:NH1	2.33	0.44
1:A:256:LEU:HB3	1:A:317:GLN:CB	2.48	0.44
1:A:86:SER:O	1:A:90:MET:HG3	2.18	0.43
1:A:727:TYR:HH	2:A:804:BOG:HO6	1.64	0.42
1:A:299:ASP:N	1:A:299:ASP:OD1	2.51	0.42
1:A:664:THR:CB	1:A:665:PRO:CD	2.95	0.42
1:A:665:PRO:HG2	1:A:666:TYR:CE2	2.54	0.42
1:A:59:ASP:OD1	1:A:605:GLN:NE2	2.51	0.42
1:A:529:LEU:HD12	1:A:529:LEU:HA	1.87	0.41
1:A:606:LEU:C	1:A:606:LEU:CD1	2.85	0.41
1:A:487:MET:CE	1:A:489:LYS:HE3	2.49	0.40
1:A:494:PRO:HG2	1:A:512:TYR:CE2	2.49	0.40
1:A:194:VAL:HG11	2:A:804:BOG:H7'1	2.03	0.40
1:A:322:TRP:CE2	1:A:388:GLY:HA3	2.56	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	670/693 (97%)	655 (98%)	15 (2%)	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	572/587 (97%)	565 (99%)	7 (1%)	71 76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	258	THR
1	A	267	ARG
1	A	578	GLU
1	A	606	LEU
1	A	634	MET
1	A	666	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	75	GLN
1	A	87	GLN
1	A	94	GLN
1	A	323	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	HWS	A	806	-	54,59,60	3.50	19 (35%)	49,89,91	2.11	11 (22%)
2	BOG	A	802	-	20,20,20	0.36	0	25,25,25	0.79	0
2	BOG	A	801	-	20,20,20	0.39	0	25,25,25	0.89	1 (4%)
2	BOG	A	803	-	20,20,20	0.43	0	25,25,25	0.67	0
2	BOG	A	804	-	20,20,20	0.43	0	25,25,25	1.12	2 (8%)
2	BOG	A	805	-	20,20,20	0.44	0	25,25,25	0.83	1 (4%)

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	HWS	A	806	-	3/3/16/23	12/48/118/120	0/3/6/6
2	BOG	A	802	-	-	7/11/31/31	0/1/1/1
2	BOG	A	801	-	-	4/11/31/31	0/1/1/1
2	BOG	A	803	-	-	4/11/31/31	0/1/1/1
2	BOG	A	804	-	-	0/11/31/31	0/1/1/1
2	BOG	A	805	-	-	0/11/31/31	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	HWS	O8-FE	-9.77	1.76	2.04
3	A	806	HWS	O7-N4	-9.52	1.21	1.38
3	A	806	HWS	O2-FE	-7.76	1.82	1.99
3	A	806	HWS	O3-C6	7.58	1.44	1.28
3	A	806	HWS	O8-C17	7.47	1.44	1.28
3	A	806	HWS	O12-C28	7.46	1.44	1.28
3	A	806	HWS	O2-N1	-7.42	1.25	1.38
3	A	806	HWS	O6-C23	5.61	1.44	1.33
3	A	806	HWS	O11-N5	-5.26	1.29	1.38
3	A	806	HWS	O12-FE	-4.70	1.91	2.04
3	A	806	HWS	O3-FE	-4.23	1.92	2.04
3	A	806	HWS	O11-FE	-3.56	1.91	1.99
3	A	806	HWS	O7-FE	-2.98	1.92	1.99
3	A	806	HWS	C5-N1	-2.66	1.42	1.47
3	A	806	HWS	C2-N2	-2.58	1.42	1.46
3	A	806	HWS	O4-C7	-2.51	1.18	1.23
3	A	806	HWS	C8-C7	-2.47	1.46	1.52
3	A	806	HWS	C7-N2	-2.40	1.29	1.33
3	A	806	HWS	O1-C1	-2.29	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	HWS	O11-N5-C27	5.77	123.77	114.13
3	A	806	HWS	O2-N1-C5	4.91	122.33	114.13
3	A	806	HWS	O6-C23-C24	4.79	123.23	111.59
3	A	806	HWS	O7-N4-C11	4.69	121.97	114.13
3	A	806	HWS	C20-C19-C18	-4.37	116.47	125.85
3	A	806	HWS	O6-C23-O10	-4.05	116.46	124.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	HWS	C26-C27-N5	3.73	118.57	110.88
3	A	806	HWS	C21-O6-C23	3.62	124.24	116.58
2	A	804	BOG	C3-C4-C5	2.92	115.45	110.24
3	A	806	HWS	O6-C21-C20	2.90	114.27	108.18
3	A	806	HWS	C19-C18-C17	2.86	127.39	123.23
2	A	801	BOG	C6-C5-C4	-2.80	106.44	113.00
3	A	806	HWS	C9-C8-N3	2.61	116.34	110.95
2	A	805	BOG	C6-C5-C4	-2.33	107.55	113.00
2	A	804	BOG	C4-C3-C2	2.18	114.64	110.82

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	806	HWS	N1
3	A	806	HWS	N5
3	A	806	HWS	N4

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	BOG	C2'-C1'-O1-C1
3	A	806	HWS	N2-C2-C3-C4
3	A	806	HWS	N3-C8-C9-C10
3	A	806	HWS	N4-C17-C18-C19
3	A	806	HWS	O8-C17-C18-C19
3	A	806	HWS	C30-C31-C32-O9
3	A	806	HWS	O10-C23-O6-C21
3	A	806	HWS	C24-C23-O6-C21
2	A	801	BOG	C4-C5-C6-O6
2	A	801	BOG	O1-C1'-C2'-C3'
2	A	801	BOG	O5-C5-C6-O6
2	A	802	BOG	C3'-C4'-C5'-C6'
2	A	803	BOG	C4'-C5'-C6'-C7'
3	A	806	HWS	C9-C10-C11-N4
2	A	802	BOG	C2'-C1'-O1-C1
2	A	802	BOG	O5-C5-C6-O6
2	A	802	BOG	C4'-C5'-C6'-C7'
3	A	806	HWS	O13-C34-N6-C24
2	A	802	BOG	O5-C1-O1-C1'
2	A	802	BOG	C2-C1-O1-C1'
2	A	801	BOG	C2'-C3'-C4'-C5'
3	A	806	HWS	C35-C34-N6-C24

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Mol	Chain	Res	Type	Atoms
2	A	802	BOG	C2'-C3'-C4'-C5'
3	A	806	HWS	C25-C26-C27-N5
3	A	806	HWS	C33-C30-C31-C32
2	A	803	BOG	C1'-C2'-C3'-C4'
2	A	803	BOG	C2'-C3'-C4'-C5'

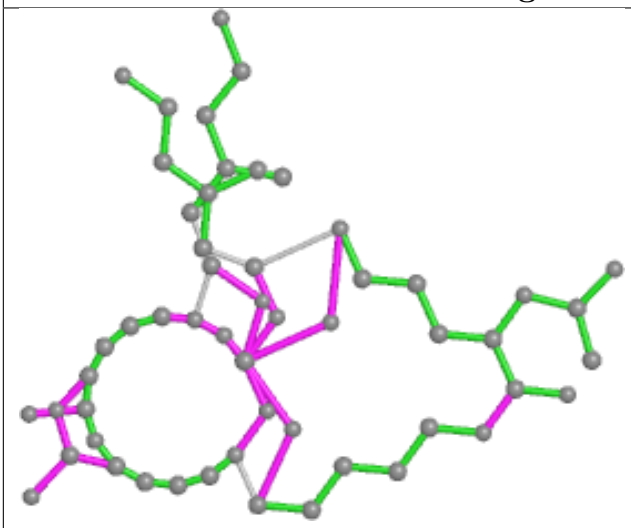
There are no ring outliers.

1 monomer is involved in 2 short contacts:

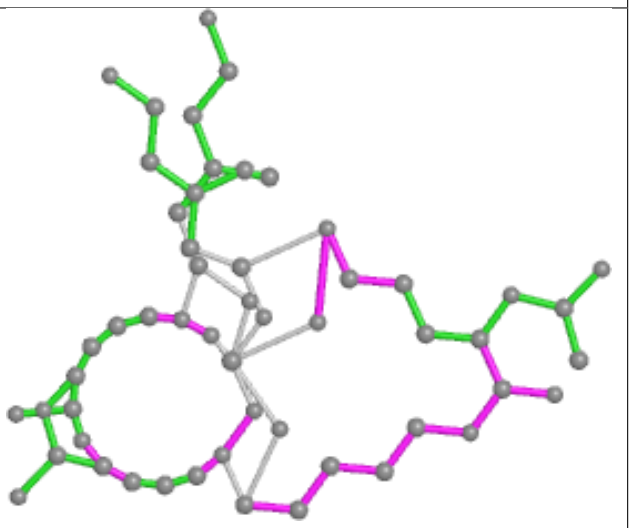
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	BOG	2	0

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

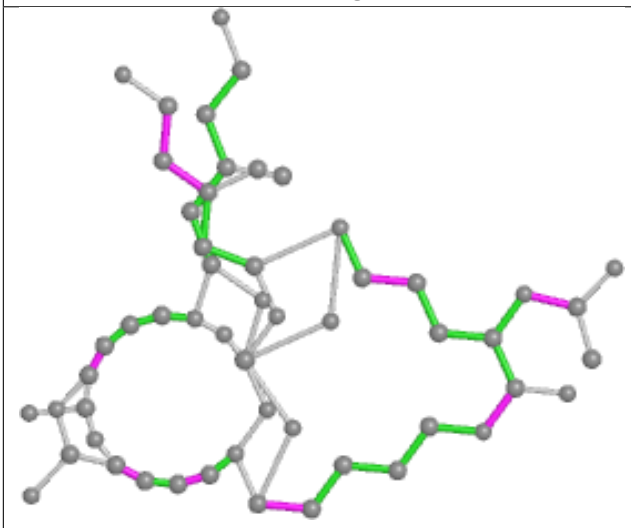
Ligand HWS A 806



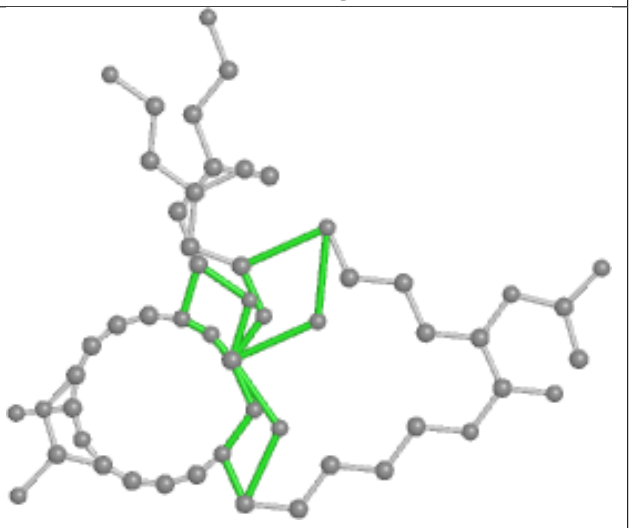
Bond lengths



Bond angles

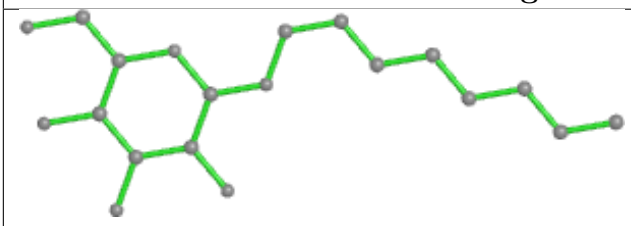


Torsions

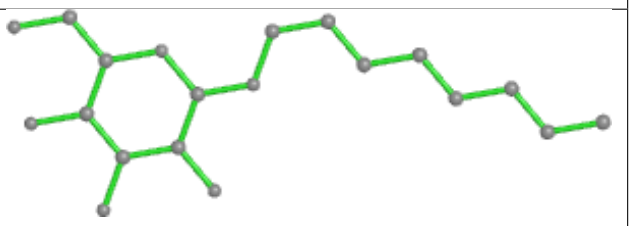


Rings

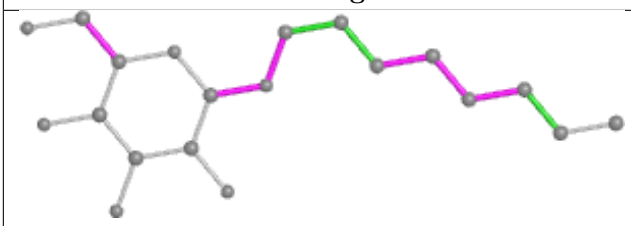
Ligand BOG A 802



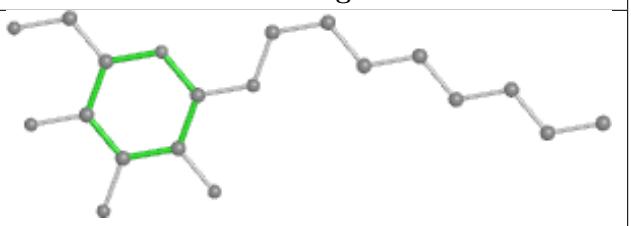
Bond lengths



Bond angles

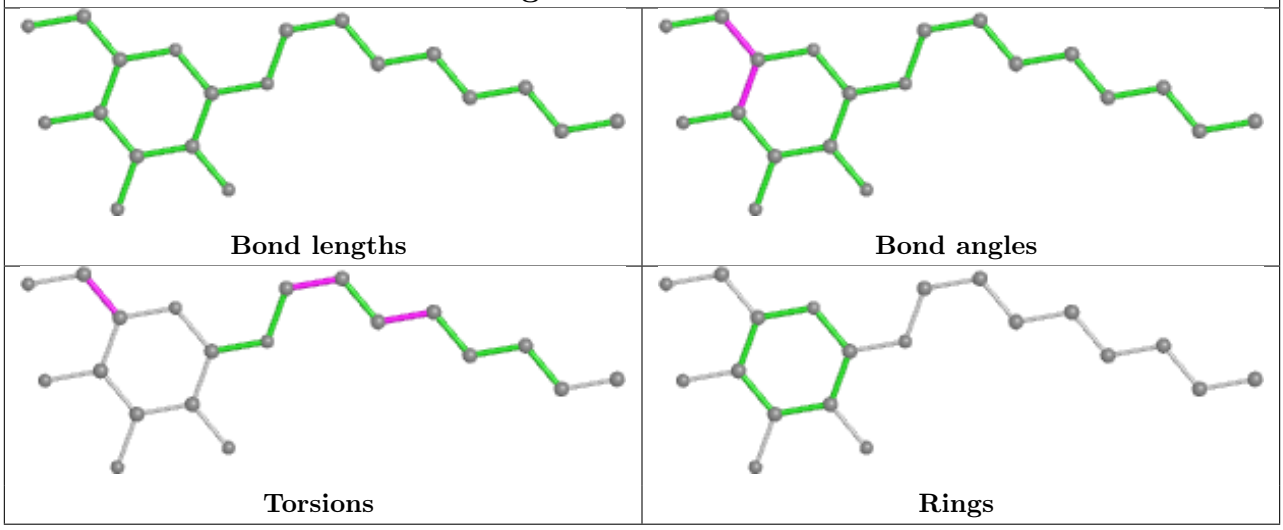


Torsions

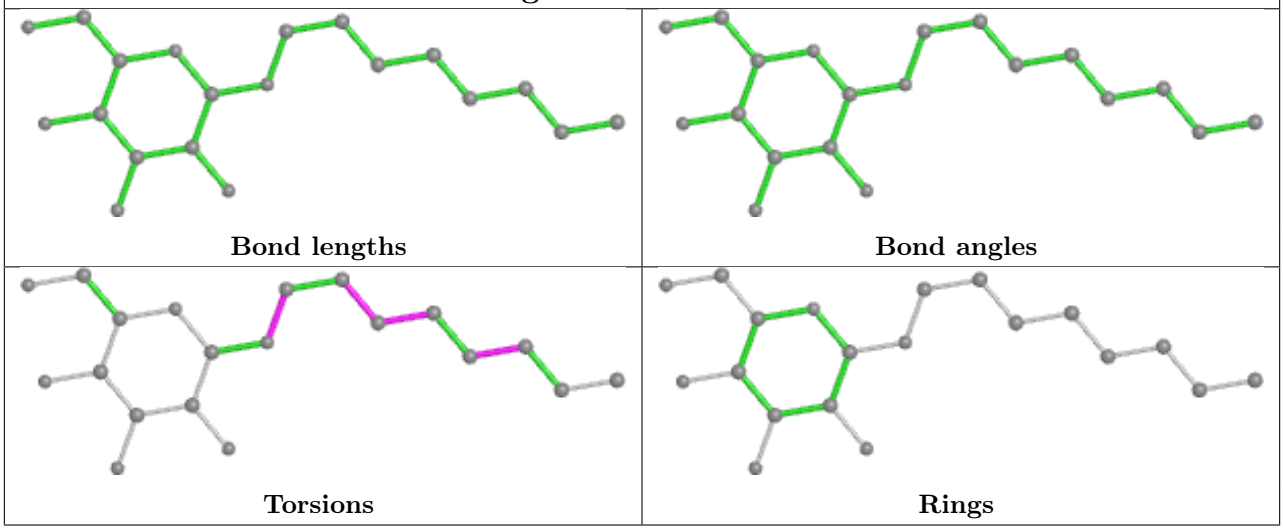


Rings

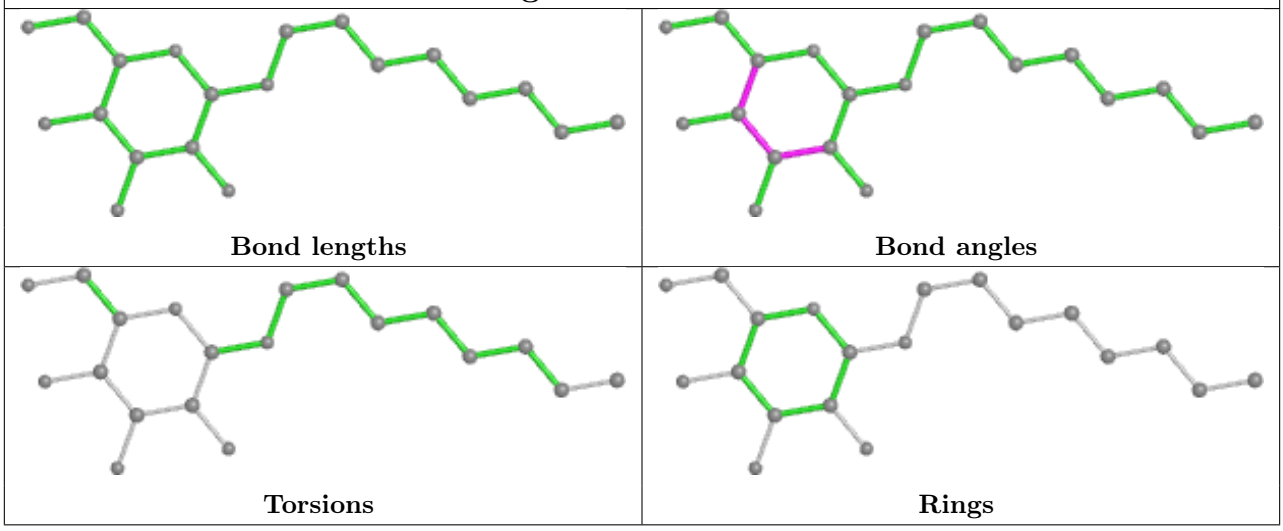
Ligand BOG A 801



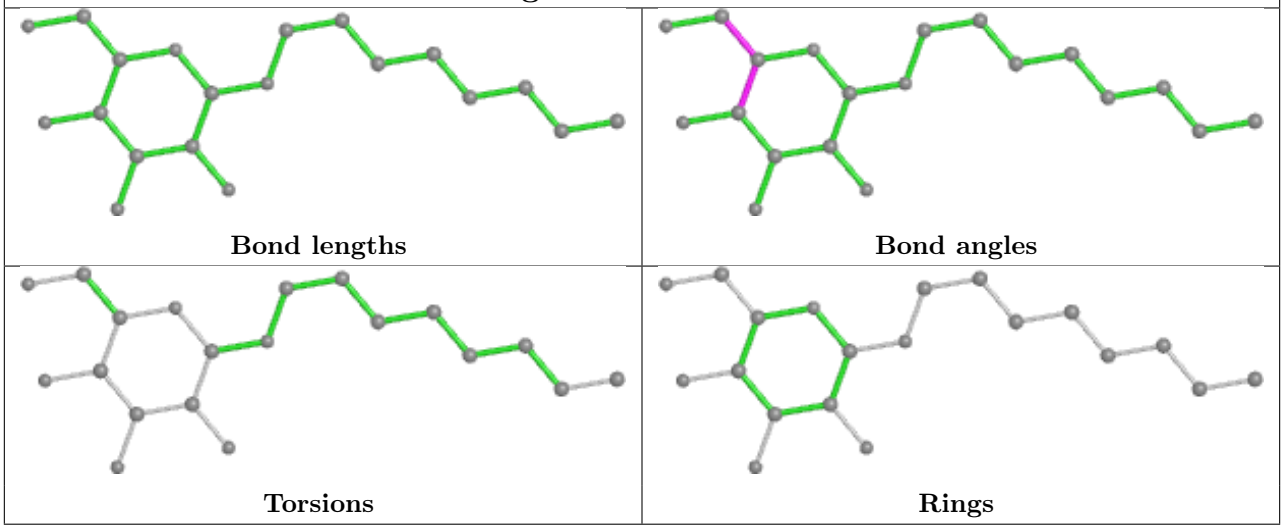
Ligand BOG A 803



Ligand BOG A 804



Ligand BOG A 805



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	672/693 (96%)	1.06	97 (14%)	2 2	23, 38, 68, 101	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	16.1
1	A	574	GLY	14.5
1	A	570	THR	11.5
1	A	319	ALA	11.5
1	A	573	PRO	10.3
1	A	580	ALA	8.7
1	A	669	PHE	8.4
1	A	321	THR	8.3
1	A	254	GLY	8.3
1	A	320	ASP	7.7
1	A	527	LYS	7.5
1	A	579	THR	7.4
1	A	666	TYR	7.1
1	A	524	SER	7.1
1	A	572	ILE	6.6
1	A	528	TYR	6.0
1	A	256	LEU	6.0
1	A	316	GLN	5.8
1	A	665	PRO	5.7
1	A	484	THR	5.6
1	A	575	SER	5.1
1	A	323	GLN	5.1
1	A	571	PRO	5.0
1	A	322	TRP	4.9
1	A	433	ASN	4.9
1	A	522	ARG	4.8
1	A	255	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	526	GLY	4.6
1	A	577	GLY	4.4
1	A	525	SER	4.3
1	A	285	GLY	4.3
1	A	489	LYS	4.1
1	A	569	GLY	4.1
1	A	487	MET	4.0
1	A	578	GLU	4.0
1	A	664	THR	3.9
1	A	324	ALA	3.8
1	A	281	TRP	3.8
1	A	359	ASN	3.8
1	A	317	GLN	3.7
1	A	479	ARG	3.6
1	A	488	GLU	3.6
1	A	486	SER	3.5
1	A	567	SER	3.5
1	A	386	ALA	3.4
1	A	520	ASN	3.4
1	A	357	TYR	3.4
1	A	568	THR	3.2
1	A	576	ASN	3.2
1	A	581	TYR	3.2
1	A	604	TRP	3.1
1	A	668	THR	3.1
1	A	352	MET	3.0
1	A	178	ILE	3.0
1	A	449	THR	2.9
1	A	485	TYR	2.9
1	A	662	THR	2.9
1	A	346	VAL	2.8
1	A	390	TYR	2.8
1	A	253	LEU	2.8
1	A	701	PHE	2.7
1	A	603	ASN	2.7
1	A	387	ASP	2.7
1	A	480	VAL	2.6
1	A	429	ASN	2.6
1	A	667	GLY	2.6
1	A	67	ALA	2.6
1	A	283	THR	2.6
1	A	393	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	284	ASP	2.5
1	A	424	ILE	2.5
1	A	345	TYR	2.5
1	A	360	TYR	2.4
1	A	69	THR	2.4
1	A	430	PHE	2.4
1	A	483	LEU	2.4
1	A	641	PRO	2.4
1	A	347	ASN	2.3
1	A	405	TYR	2.3
1	A	391	GLU	2.3
1	A	71	MET	2.3
1	A	729	PHE	2.3
1	A	187	SER	2.3
1	A	389	SER	2.2
1	A	523	ASP	2.2
1	A	130	TYR	2.2
1	A	314	LEU	2.2
1	A	663	VAL	2.2
1	A	218	GLY	2.2
1	A	396	GLN	2.1
1	A	451	HIS	2.1
1	A	394	GLY	2.1
1	A	448	ASP	2.0
1	A	259	LEU	2.0
1	A	728	GLN	2.0
1	A	545	TRP	2.0
1	A	432	GLY	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,

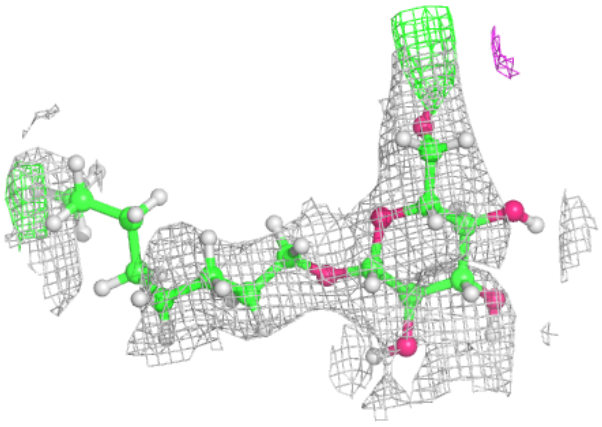
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

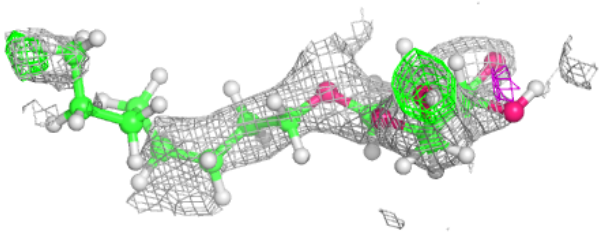
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BOG	A	803	20/20	0.75	0.31	64,94,108,127	0
2	BOG	A	804	20/20	0.78	0.22	58,83,126,131	0
2	BOG	A	802	20/20	0.89	0.18	59,67,75,85	0
2	BOG	A	805	20/20	0.89	0.24	70,87,108,115	0
3	HWS	A	806	54/55	0.94	0.15	26,36,50,52	0
2	BOG	A	801	20/20	0.97	0.14	39,50,58,83	0

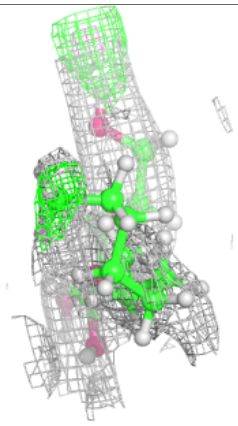
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG A 803:

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

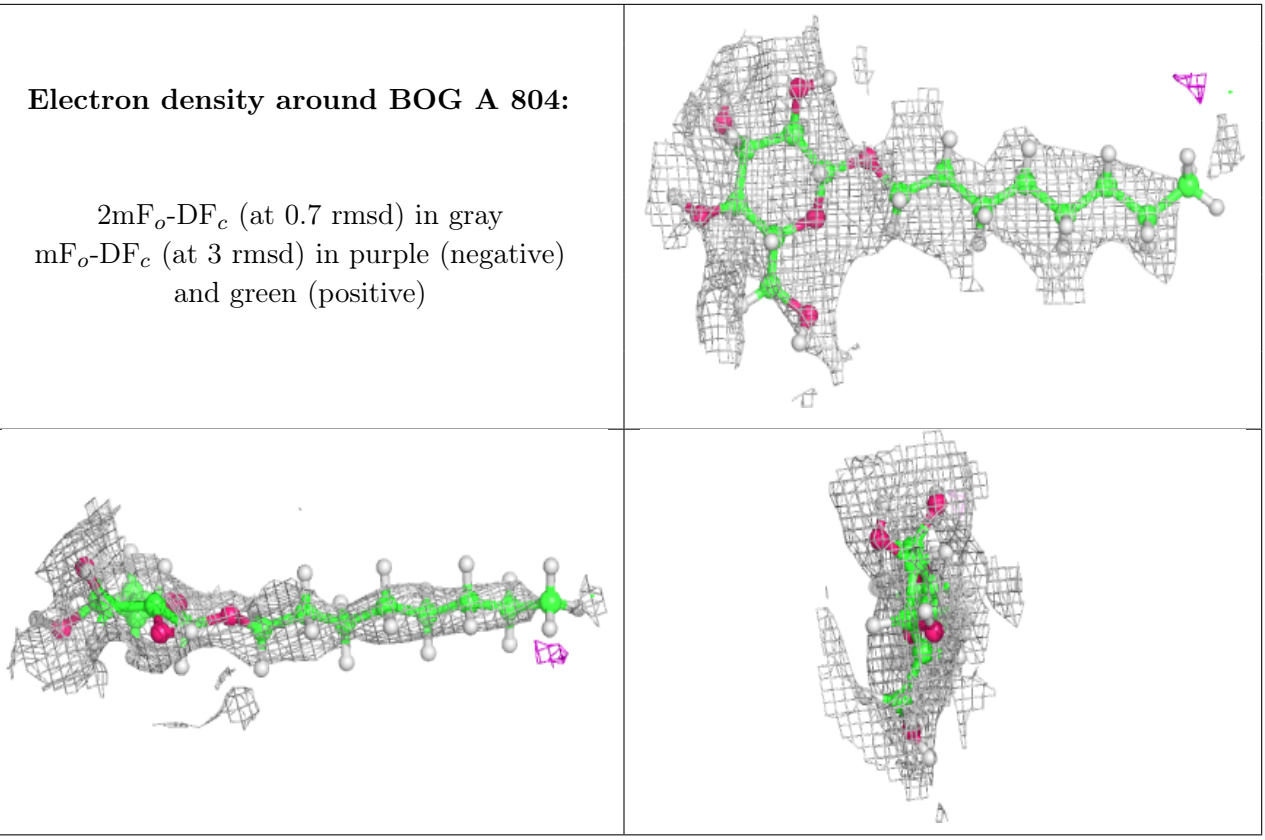






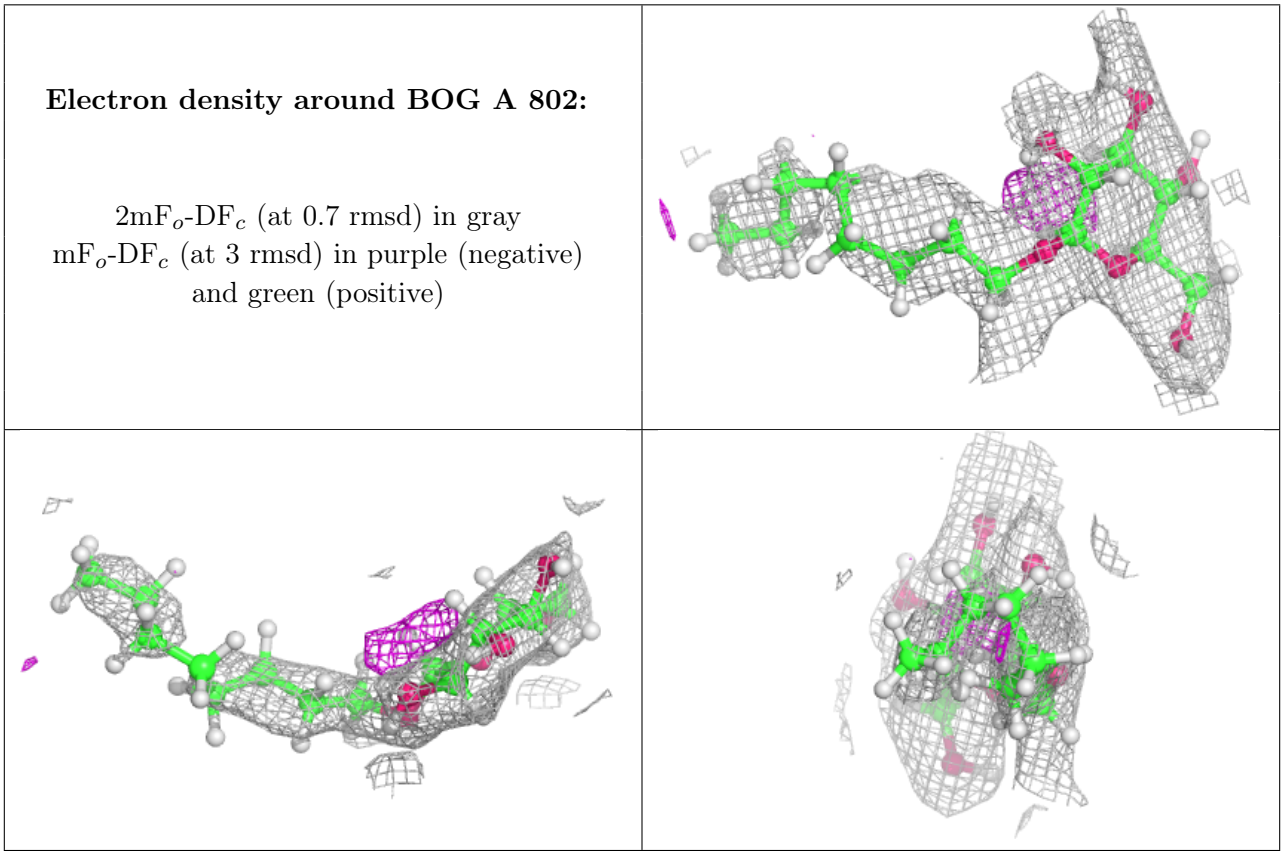
Electron density around BOG A 804:

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



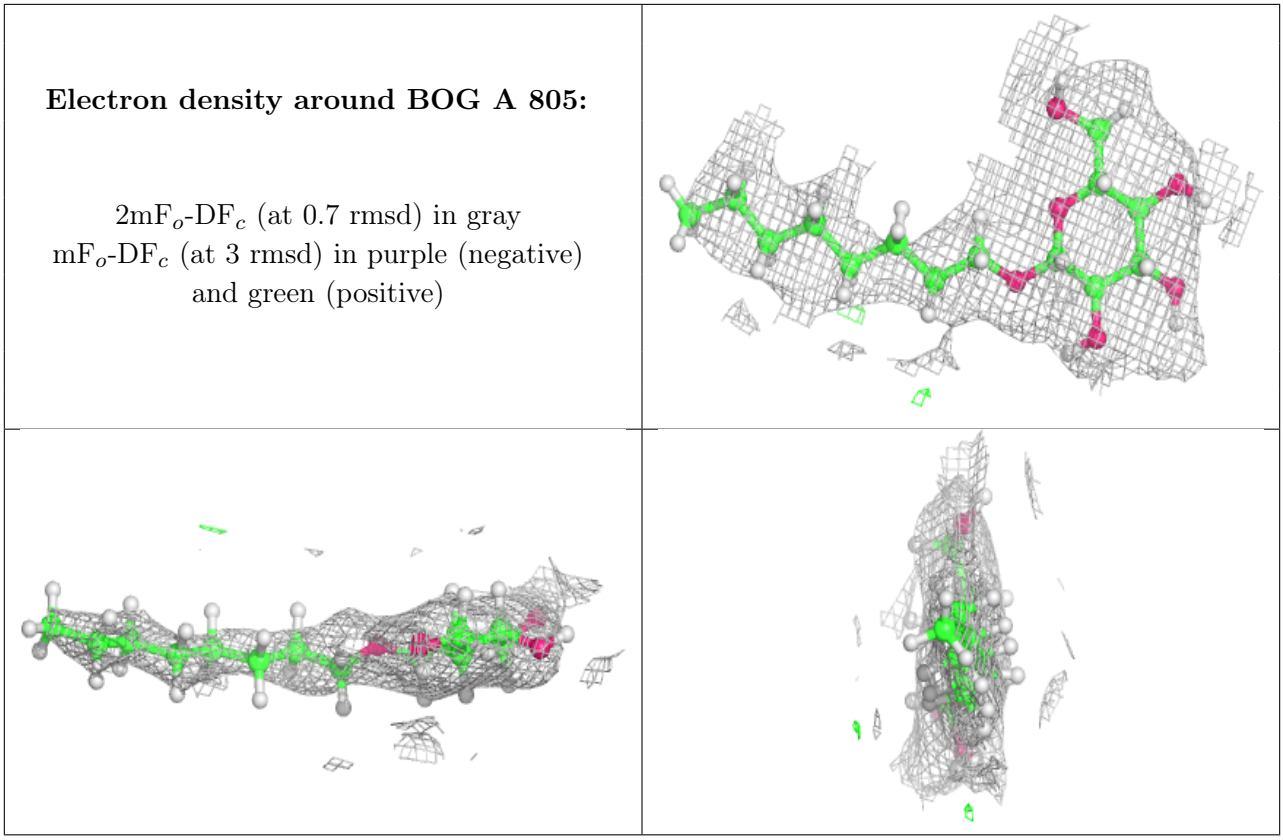
Electron density around BOG A 802:

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



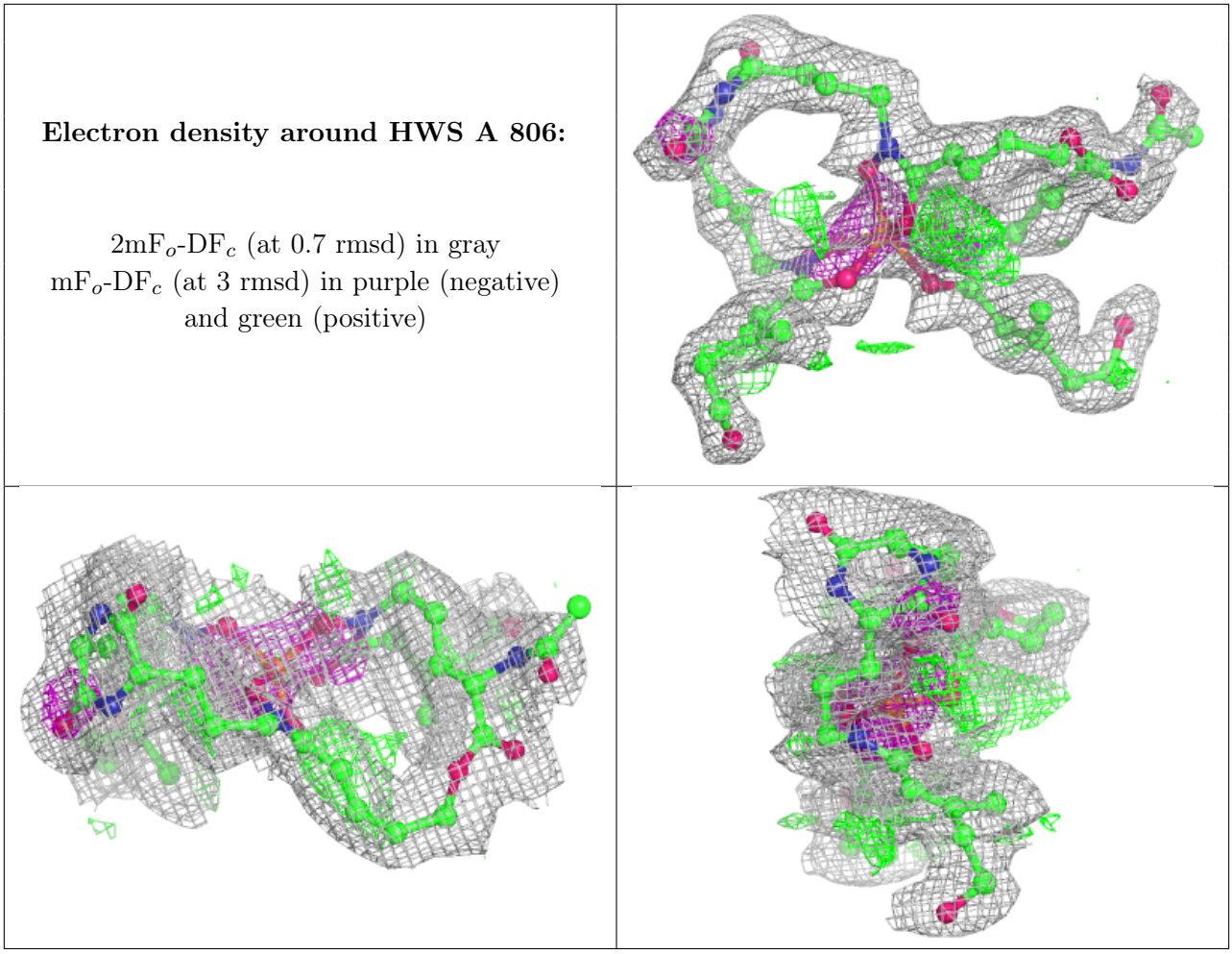
Electron density around BOG A 805:

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



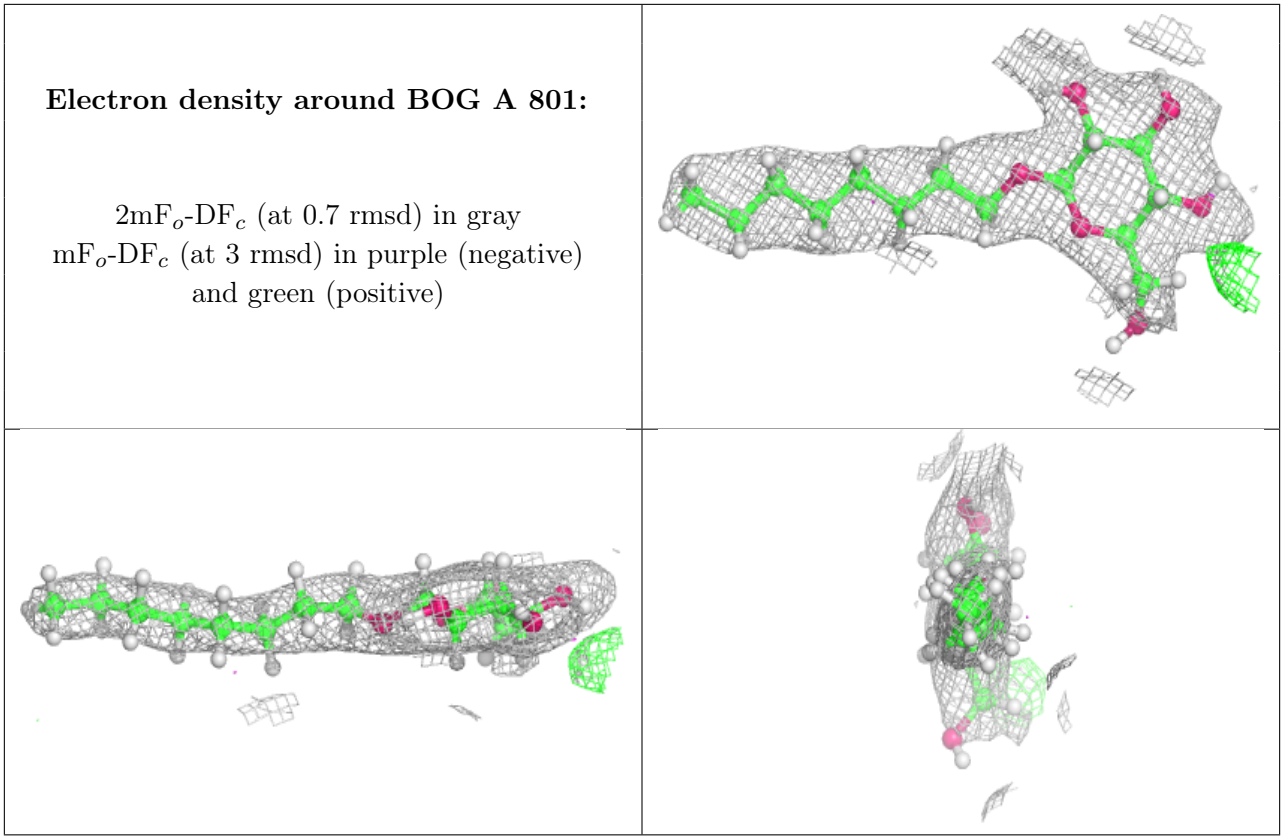
Electron density around HWS A 806:

$2mF_o$-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 801:

$2mF_o$-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.