Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 05:10 PM EDT

PDB ID	:	6D9Z
Title	:	Structure of CysZ, a sulfate permease from Pseudomonas Denitrificans
Authors	:	Sanghai, Z.A.; Clarke, O.B.; Liu, Q.; Banerjee, S.; Rajashankar, K.R.; Hendrickson, W.A.; Mancia, F.
Deposited on	:	2018-04-30
Resolution	:	3.40 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 (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:

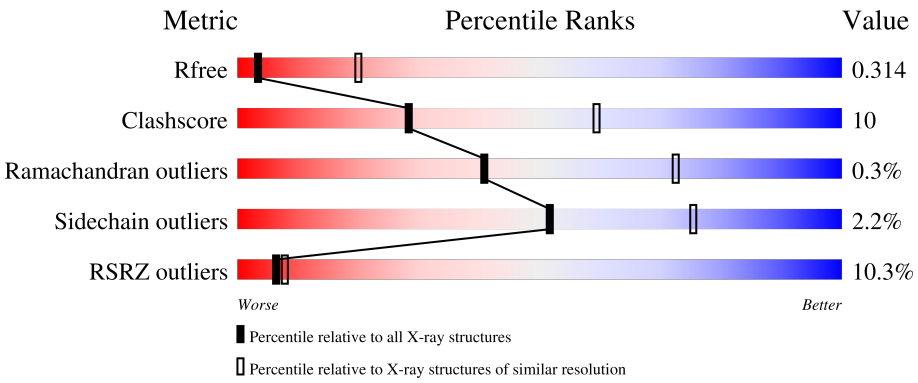
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	6% 70% 24%
1	B	246	20% 72% 23%
1	C	246	7% 71% 26%
1	D	246	15% 78% 19%
1	E	246	5% 76% 21%

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Mol	Chain	Length	Quality of chain
1	F	246	6% 76% 22%

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	A	305	-	-	-	X
2	BOG	B	302	-	-	-	X
2	BOG	C	302	-	-	-	X
2	BOG	C	303	-	-	-	X
2	BOG	D	302	-	-	-	X
2	BOG	E	301	-	-	-	X
2	BOG	E	302	-	-	-	X
2	BOG	F	301	-	-	-	X
2	BOG	F	305	-	-	-	X

2 Entry composition (i)

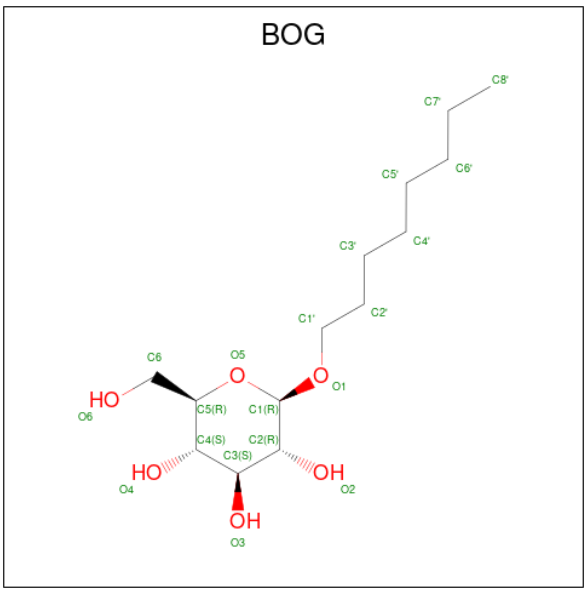
There are 2 unique types of molecules in this entry. The entry contains 24189 atoms, of which 12374 are hydrogens and 0 are deuteriums.

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 Sulfate transporter CysZ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	F	240	3894	1303	1976	303	301	11	0	0	0
1	A	236	3862	1290	1969	298	294	11	0	0	0
1	B	236	3850	1284	1963	298	294	11	0	0	0
1	C	241	3918	1306	1994	304	303	11	0	0	0
1	D	240	3850	1292	1952	296	299	11	0	0	0
1	E	240	3855	1288	1960	298	298	11	0	0	0

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



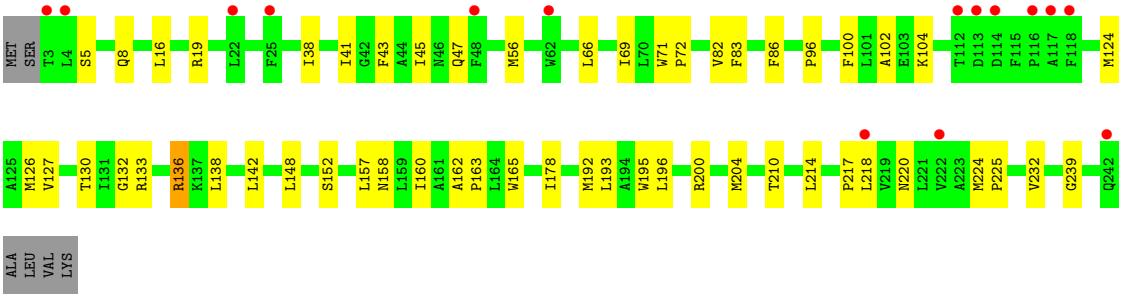
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	F	1	48	14	28	6	0	0
			Total	C	H	O		
2	F	1	48	14	28	6	0	0
			Total	C	H	O		
2	F	1	48	14	28	6	0	0
			Total	C	H	O		
2	F	1	48	14	28	6	0	0
			Total	C	H	O		
2	F	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	A	1	48	14	28	6	0	0
			Total	C	H	O		
2	B	1	48	14	28	6	0	0
			Total	C	H	O		
2	B	1	48	14	28	6	0	0
			Total	C	H	O		
2	C	1	48	14	28	6	0	0
			Total	C	H	O		
2	C	1	48	14	28	6	0	0
			Total	C	H	O		
2	C	1	48	14	28	6	0	0
			Total	C	H	O		
2	D	1	48	14	28	6	0	0
			Total	C	H	O		
2	D	1	48	14	28	6	0	0
			Total	C	H	O		
2	E	1	48	14	28	6	0	0
			Total	C	H	O		
2	E	1	48	14	28	6	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.

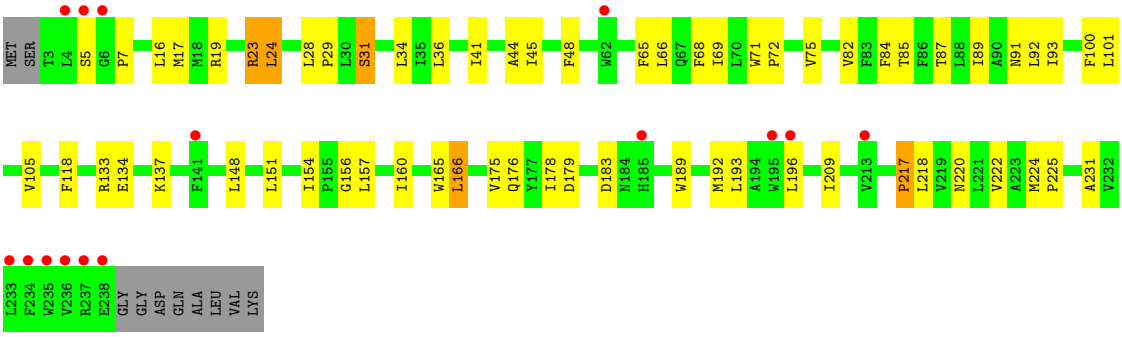
• Molecule 1: Sulfate transporter CysZ

Chain F:



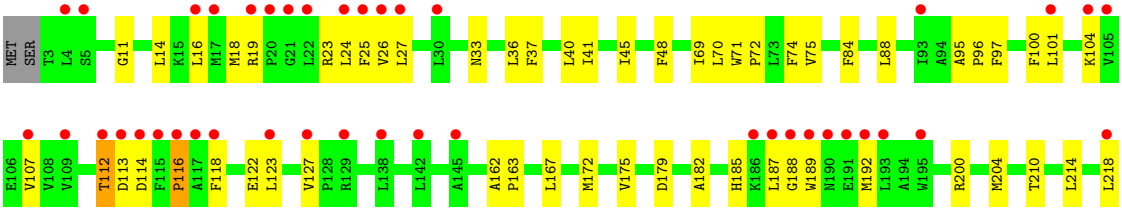
• Molecule 1: Sulfate transporter CysZ

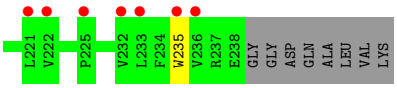
Chain A:



• Molecule 1: Sulfate transporter CysZ

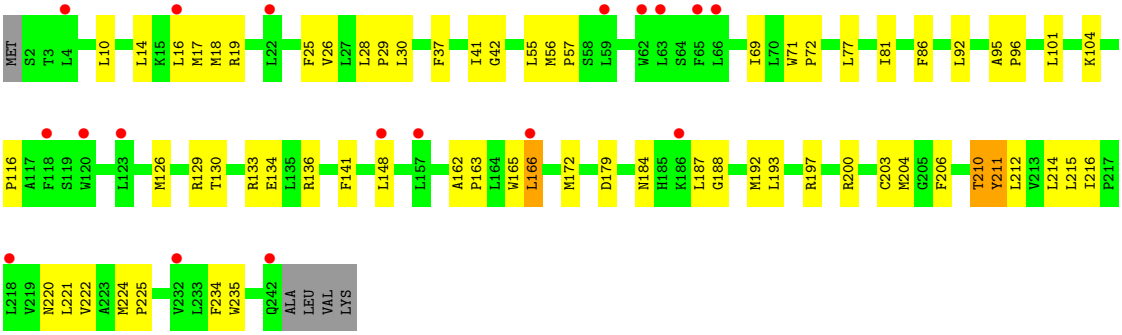
Chain B:





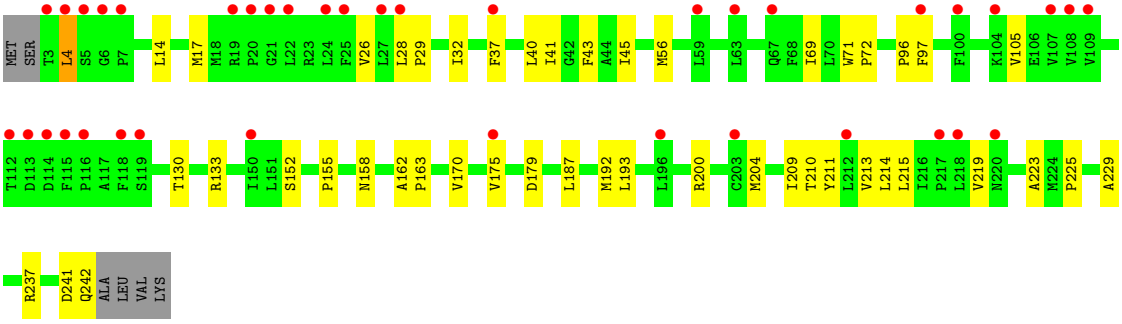
• Molecule 1: Sulfate transporter CysZ

Chain C:



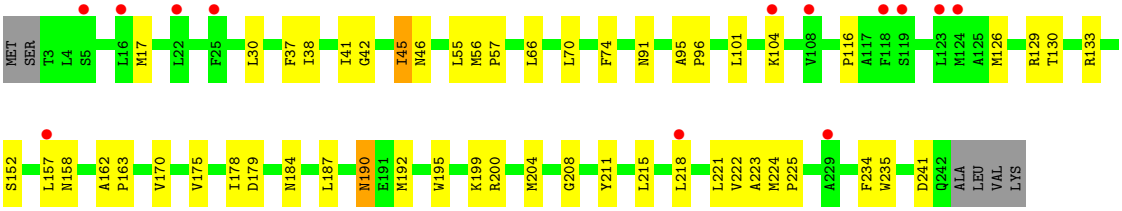
• Molecule 1: Sulfate transporter CysZ

Chain D:



• Molecule 1: Sulfate transporter CysZ

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	225.13Å 225.13Å 96.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.40 86.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.40) 89.7 (86.57-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 3.41Å)	Xtriage
Refinement program	phenix.refine 1.11.1_2575	Depositor
R, R_{free}	0.245 , 0.289 0.264 , 0.314	Depositor DCC
R_{free} test set	1948 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	159.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 113.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24189	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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 (i)

5.1 Standard geometry (i)

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	0.48	0/1955	0.59	0/2672
1	B	0.42	0/1948	0.52	0/2663
1	C	0.49	0/1986	0.58	0/2713
1	D	0.39	0/1960	0.52	0/2682
1	E	0.45	0/1955	0.54	0/2672
1	F	0.51	0/1980	0.60	2/2705 (0.1%)
All	All	0.46	0/11784	0.56	2/16107 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	136	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	F	136	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	1893	1969	1971	45	0
1	B	1887	1963	1964	42	0
1	C	1924	1994	1994	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1898	1952	1952	36	0
1	E	1895	1960	1960	36	0
1	F	1918	1976	1989	34	0
2	A	120	168	168	12	0
2	B	40	56	55	5	0
2	C	60	84	84	2	0
2	D	40	56	56	4	0
2	E	40	56	56	3	0
2	F	100	140	140	7	0
All	All	11815	12374	12389	237	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.

All (237) 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:D:302:BOG:H8'1	1:E:223:ALA:HA	1.63	0.80
1:A:23:ARG:NH2	2:A:301:BOG:O6	2.15	0.79
1:A:7:PRO:HB2	1:A:209:ILE:HG21	1.71	0.72
1:A:220:ASN:ND2	2:A:305:BOG:O4	2.22	0.71
1:B:69:ILE:O	1:B:72:PRO:HD2	1.93	0.69
1:E:126:MET:O	1:E:130:THR:HG22	1.97	0.64
1:D:200:ARG:O	1:D:204:MET:HB2	1.97	0.64
1:D:219:VAL:HG12	1:D:223:ALA:HB2	1.81	0.62
1:A:133:ARG:NE	1:A:183:ASP:OD1	2.30	0.62
1:B:84:PHE:HB3	2:B:302:BOG:C6'	2.30	0.62
1:B:33:ASN:O	1:B:37:PHE:CB	2.48	0.61
1:E:200:ARG:O	1:E:204:MET:HB2	2.00	0.61
2:B:302:BOG:H8'3	2:B:302:BOG:H4'2	1.82	0.61
1:C:56:MET:HE1	1:C:71:TRP:HA	1.83	0.61
1:E:17:MET:HE1	1:E:101:LEU:HD21	1.82	0.60
1:C:200:ARG:O	1:C:204:MET:HB2	2.02	0.60
1:B:179:ASP:HB2	1:B:192:MET:HE1	1.83	0.59
1:F:83:PHE:CE1	2:F:302:BOG:H1'2	2.37	0.59
1:A:16:LEU:O	1:A:19:ARG:HG2	2.03	0.58
1:A:17:MET:O	1:A:23:ARG:HB3	2.04	0.57
1:A:28:LEU:CB	1:A:29:PRO:HD3	2.35	0.57
1:A:224:MET:HB2	1:A:225:PRO:HD3	1.86	0.57
1:C:133:ARG:NH1	1:C:179:ASP:OD1	2.37	0.57
1:C:220:ASN:OD1	1:C:221:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ASN:O	2:E:301:BOG:O6	2.14	0.56
1:F:86:PHE:CD2	2:F:302:BOG:H2'1	2.41	0.56
1:C:17:MET:HE1	1:C:101:LEU:HD21	1.88	0.56
1:E:133:ARG:NH1	1:E:179:ASP:OD1	2.39	0.56
1:F:152:SER:O	1:F:158:ASN:HB3	2.05	0.56
1:F:71:TRP:HB3	1:F:72:PRO:HD3	1.88	0.55
1:B:200:ARG:O	1:B:204:MET:HB2	2.06	0.55
1:B:189:TRP:O	1:B:192:MET:HG2	2.06	0.54
1:C:187:LEU:HD23	1:C:188:GLY:N	2.23	0.54
1:A:7:PRO:CB	1:A:209:ILE:HG21	2.37	0.54
1:C:126:MET:O	1:C:130:THR:HG22	2.07	0.54
1:B:33:ASN:O	1:B:37:PHE:HB2	2.08	0.53
1:B:18:MET:O	1:B:23:ARG:NH2	2.42	0.53
2:E:301:BOG:H7'1	2:E:301:BOG:H3'2	1.89	0.53
1:E:96:PRO:HA	1:E:130:THR:HG21	1.90	0.53
1:F:200:ARG:O	1:F:204:MET:HB2	2.09	0.53
1:D:37:PHE:CE1	1:E:218:LEU:HB3	2.44	0.53
1:D:14:LEU:HD21	2:E:301:BOG:H2'2	1.91	0.52
1:B:187:LEU:HD23	1:B:188:GLY:N	2.24	0.52
1:C:133:ARG:NH2	1:C:187:LEU:O	2.35	0.52
1:B:182:ALA:HB1	1:B:187:LEU:CD1	2.40	0.52
1:C:148:LEU:HD13	1:C:165:TRP:HA	1.91	0.52
1:E:179:ASP:HA	1:E:192:MET:HE3	1.91	0.52
1:E:30:LEU:HD13	1:E:221:LEU:HD13	1.92	0.52
1:B:95:ALA:HB3	1:B:96:PRO:HD3	1.92	0.52
1:B:25:PHE:CD2	1:B:101:LEU:CD1	2.93	0.51
1:B:33:ASN:O	1:B:37:PHE:HB3	2.11	0.51
1:E:195:TRP:CH2	1:E:199:LYS:HE3	2.45	0.51
1:B:37:PHE:O	1:B:41:ILE:HG22	2.11	0.51
1:F:56:MET:HE1	1:F:71:TRP:HA	1.93	0.51
1:F:45:ILE:HG22	2:F:301:BOG:O3	2.11	0.50
1:B:182:ALA:HB1	1:B:187:LEU:HD13	1.94	0.50
1:A:133:ARG:HH11	1:A:189:TRP:HE3	1.58	0.50
1:B:84:PHE:HB3	2:B:302:BOG:H6'2	1.94	0.50
1:E:129:ARG:NH1	1:E:184:ASN:OD1	2.44	0.50
1:B:187:LEU:HD22	1:B:192:MET:HB3	1.93	0.50
1:F:192:MET:HG3	1:F:193:LEU:N	2.26	0.50
1:C:187:LEU:HD22	1:C:192:MET:HB3	1.93	0.50
1:D:45:ILE:O	2:D:301:BOG:H2	2.12	0.50
1:C:104:LYS:HD2	1:C:116:PRO:HB2	1.95	0.49
1:D:213:VAL:CG1	1:D:219:VAL:HG11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD13	1:A:165:TRP:HA	1.95	0.49
1:B:218:LEU:HB3	1:C:37:PHE:CE1	2.47	0.49
1:F:220:ASN:O	1:F:224:MET:HG3	2.12	0.49
1:A:41:ILE:O	1:A:45:ILE:HG12	2.13	0.49
1:A:87:THR:O	1:A:91:ASN:ND2	2.46	0.49
1:B:84:PHE:O	1:B:88:LEU:N	2.36	0.49
1:D:209:ILE:O	1:D:213:VAL:HB	2.13	0.49
1:B:36:LEU:O	1:B:40:LEU:HD13	2.13	0.49
1:A:65:PHE:HA	1:A:68:PHE:HD2	1.78	0.49
1:A:157:LEU:O	1:A:160:ILE:HG22	2.13	0.48
1:F:38:ILE:HG23	2:A:302:BOG:H6'1	1.94	0.48
1:A:178:ILE:HA	1:A:231:ALA:HB1	1.95	0.48
1:B:104:LYS:HD2	1:B:116:PRO:HG3	1.95	0.48
1:C:95:ALA:HB3	1:C:96:PRO:HD3	1.95	0.48
1:F:124:MET:HA	1:F:127:VAL:HG23	1.94	0.48
1:C:96:PRO:HA	1:C:130:THR:HG21	1.95	0.48
1:E:91:ASN:O	1:E:95:ALA:N	2.47	0.48
1:C:26:VAL:O	1:C:29:PRO:HD2	2.14	0.48
1:F:43:PHE:CE2	1:F:47:GLN:HG3	2.48	0.48
1:B:70:LEU:O	1:B:74:PHE:HD1	1.97	0.48
1:C:211:TYR:CE1	1:C:215:LEU:HD21	2.49	0.48
1:D:41:ILE:O	1:D:45:ILE:HG12	2.13	0.48
1:D:152:SER:HA	1:D:158:ASN:HA	1.96	0.48
1:F:138:LEU:HD22	1:F:142:LEU:HD11	1.96	0.47
1:B:11:GLY:O	1:B:14:LEU:HB3	2.14	0.47
1:D:211:TYR:CE1	1:D:215:LEU:HD21	2.49	0.47
1:D:213:VAL:HG12	1:D:219:VAL:HG11	1.97	0.47
1:A:17:MET:O	1:A:23:ARG:HG2	2.15	0.47
1:F:41:ILE:HG12	1:A:222:VAL:HG11	1.97	0.47
1:A:100:PHE:CE2	1:A:118:PHE:HD1	2.32	0.47
1:D:152:SER:O	1:D:158:ASN:HB3	2.15	0.47
1:C:221:LEU:HD21	2:C:301:BOG:H62	1.96	0.47
1:A:175:VAL:HG12	1:A:196:LEU:HD12	1.96	0.46
1:C:210:THR:O	1:C:214:LEU:HD12	2.15	0.46
1:A:31:SER:O	1:A:34:LEU:HB2	2.15	0.46
1:D:45:ILE:HD13	2:D:301:BOG:H5'1	1.98	0.46
1:D:96:PRO:HA	1:D:130:THR:HG21	1.97	0.46
1:F:195:TRP:HH2	1:F:239:GLY:HA3	1.80	0.46
1:A:71:TRP:HB3	1:A:72:PRO:HD3	1.96	0.46
1:A:156:GLY:H	1:C:166:LEU:HD13	1.81	0.46
1:C:92:LEU:HA	1:C:134:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HD3	1:A:176:GLN:NE2	2.31	0.46
1:C:200:ARG:O	1:C:204:MET:CB	2.64	0.46
1:A:48:PHE:HZ	1:A:75:VAL:HG13	1.79	0.46
1:A:151:LEU:HD12	1:A:154:ILE:HD12	1.96	0.46
1:B:162:ALA:HB3	1:B:163:PRO:HD3	1.98	0.46
1:C:16:LEU:O	1:C:19:ARG:HG2	2.16	0.46
1:B:45:ILE:CD1	1:C:222:VAL:HG11	2.46	0.46
1:D:133:ARG:NH1	1:D:179:ASP:OD1	2.49	0.46
1:E:38:ILE:O	1:E:41:ILE:HG22	2.16	0.46
1:D:56:MET:HE2	1:D:71:TRP:HA	1.98	0.45
1:F:210:THR:O	1:F:214:LEU:HB2	2.16	0.45
1:B:71:TRP:HB3	1:B:72:PRO:HD3	1.98	0.45
1:B:107:VAL:HB	1:B:112:THR:HB	1.98	0.45
1:A:36:LEU:HD22	1:A:93:ILE:HD12	1.99	0.45
1:A:84:PHE:CG	2:A:303:BOG:H4'1	2.51	0.45
1:C:69:ILE:O	1:C:72:PRO:HD2	2.17	0.45
1:C:77:LEU:CD2	1:E:70:LEU:HD21	2.46	0.45
1:C:129:ARG:NH1	1:C:184:ASN:OD1	2.49	0.45
1:E:162:ALA:HB3	1:E:163:PRO:HD3	1.98	0.45
1:A:92:LEU:HA	1:A:134:GLU:OE1	2.17	0.45
1:C:141:PHE:CD1	1:C:172:MET:HG2	2.52	0.45
1:D:40:LEU:O	1:D:43:PHE:HB3	2.17	0.45
1:D:69:ILE:O	1:D:72:PRO:HD2	2.17	0.45
1:B:16:LEU:O	1:B:19:ARG:HG2	2.17	0.45
1:B:18:MET:O	1:B:23:ARG:CZ	2.64	0.45
1:C:71:TRP:HB3	1:C:72:PRO:HD3	1.99	0.45
1:F:148:LEU:HD13	1:F:165:TRP:HA	1.99	0.45
1:C:86:PHE:CG	2:C:301:BOG:H4'2	2.52	0.45
1:A:217:PRO:O	2:A:305:BOG:O3	2.28	0.44
1:F:82:VAL:HG12	2:F:302:BOG:H6'1	1.99	0.44
1:F:162:ALA:HB3	1:F:163:PRO:HD3	2.00	0.44
1:A:220:ASN:O	1:A:224:MET:HG3	2.18	0.44
1:B:118:PHE:CD2	1:B:118:PHE:C	2.91	0.44
1:E:37:PHE:O	1:E:41:ILE:HG22	2.18	0.44
1:F:126:MET:O	1:F:130:THR:HG22	2.18	0.44
1:C:41:ILE:HG23	1:C:42:GLY:N	2.33	0.44
1:D:241:ASP:C	1:D:242:GLN:HG3	2.37	0.44
1:A:101:LEU:O	1:A:105:VAL:HG23	2.18	0.44
1:B:210:THR:O	1:B:214:LEU:HB2	2.18	0.44
1:C:192:MET:HG3	1:C:193:LEU:N	2.32	0.44
1:D:26:VAL:HG13	1:D:225:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HB2	1:D:29:PRO:HD3	2.00	0.44
1:D:210:THR:O	1:D:214:LEU:HB2	2.17	0.44
2:B:301:BOG:H1	2:B:302:BOG:O2	2.18	0.44
1:C:162:ALA:HB3	1:C:163:PRO:HD3	2.00	0.44
1:D:41:ILE:HG12	1:E:222:VAL:HG11	1.99	0.44
1:D:105:VAL:HG11	1:D:229:ALA:HA	2.00	0.44
1:C:14:LEU:O	1:C:18:MET:HG3	2.18	0.43
1:C:206:PHE:O	1:C:210:THR:OG1	2.33	0.43
1:F:83:PHE:CD1	2:F:302:BOG:H1'2	2.53	0.43
1:A:66:LEU:O	1:A:69:ILE:HG22	2.17	0.43
1:C:55:LEU:HA	1:E:57:PRO:HG3	1.99	0.43
1:D:192:MET:HG3	1:D:193:LEU:N	2.32	0.43
1:F:157:LEU:O	1:F:160:ILE:HG22	2.17	0.43
1:C:224:MET:HB2	1:C:225:PRO:HD3	2.00	0.43
1:A:192:MET:CG	1:A:193:LEU:N	2.81	0.43
1:E:178:ILE:HD13	1:E:234:PHE:CD1	2.53	0.43
1:D:170:VAL:HG12	1:D:204:MET:SD	2.58	0.43
2:D:301:BOG:O2	2:D:301:BOG:H5	2.19	0.43
1:D:37:PHE:O	1:D:41:ILE:HG22	2.18	0.43
1:D:219:VAL:CG1	1:D:223:ALA:HB2	2.47	0.43
2:A:302:BOG:H1'2	2:A:302:BOG:H2	1.86	0.43
1:E:170:VAL:HG13	1:E:208:GLY:N	2.33	0.43
1:A:28:LEU:HB2	1:A:29:PRO:HD3	2.00	0.43
1:C:214:LEU:HD21	1:C:224:MET:HG2	2.01	0.43
1:E:104:LYS:HD2	1:E:116:PRO:HB2	2.01	0.43
1:A:82:VAL:HG12	2:A:305:BOG:H7'1	2.01	0.43
1:F:132:GLY:O	1:F:136:ARG:HG2	2.19	0.42
1:A:7:PRO:CB	1:A:209:ILE:CG2	2.98	0.42
1:B:179:ASP:CB	1:B:192:MET:HE1	2.49	0.42
1:F:100:PHE:CZ	1:F:104:LYS:HE3	2.54	0.42
1:F:178:ILE:HG21	1:F:196:LEU:HD21	2.01	0.42
1:C:216:ILE:N	1:C:216:ILE:HD12	2.33	0.42
1:E:133:ARG:NH1	1:E:192:MET:SD	2.92	0.42
1:F:66:LEU:O	1:F:69:ILE:HG22	2.19	0.42
1:E:41:ILE:HG23	1:E:42:GLY:H	1.85	0.42
1:D:162:ALA:HB3	1:D:163:PRO:HD3	2.00	0.42
1:E:152:SER:O	1:E:158:ASN:HB3	2.19	0.42
1:A:166:LEU:CD1	1:D:155:PRO:HG2	2.50	0.42
1:B:167:LEU:HD21	1:E:157:LEU:HD21	2.00	0.42
1:C:25:PHE:HD1	1:C:28:LEU:HD11	1.84	0.42
1:C:187:LEU:HD12	1:C:235:TRP:HH2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PHE:CE2	1:B:118:PHE:HD1	2.37	0.42
1:B:123:LEU:O	1:B:127:VAL:HG23	2.19	0.42
1:B:41:ILE:O	1:B:45:ILE:HG13	2.20	0.42
1:B:48:PHE:HZ	1:B:75:VAL:HG13	1.85	0.42
1:D:4:LEU:HD22	1:D:237:ARG:HG3	2.01	0.42
1:E:41:ILE:O	1:E:45:ILE:HG13	2.20	0.42
1:A:28:LEU:CB	1:A:29:PRO:CD	2.98	0.42
1:C:41:ILE:HG23	1:C:42:GLY:H	1.85	0.42
1:F:16:LEU:O	1:F:19:ARG:HG2	2.19	0.42
1:E:190:ASN:OD1	1:E:190:ASN:N	2.53	0.42
1:E:56:MET:HA	1:E:74:PHE:HE2	1.85	0.41
1:A:24:LEU:HB3	2:A:304:BOG:H1'1	2.02	0.41
1:C:57:PRO:HB3	1:E:55:LEU:O	2.20	0.41
1:C:81:ILE:HD13	1:E:66:LEU:HD11	2.02	0.41
1:C:211:TYR:HE1	1:C:215:LEU:HD21	1.85	0.41
1:C:197:ARG:HA	1:C:200:ARG:HG3	2.03	0.41
1:C:30:LEU:HD13	1:C:221:LEU:HD13	2.02	0.41
1:D:56:MET:HE1	1:D:71:TRP:CE3	2.54	0.41
1:E:175:VAL:O	1:E:179:ASP:HB2	2.20	0.41
1:F:102:ALA:HA	1:F:232:VAL:HG21	2.01	0.41
1:A:84:PHE:CD1	2:A:303:BOG:C4'	3.03	0.41
2:A:302:BOG:H3'2	2:A:302:BOG:O5	2.20	0.41
1:B:187:LEU:HD12	1:B:235:TRP:CH2	2.56	0.41
1:B:25:PHE:CD2	1:B:101:LEU:HD13	2.56	0.41
1:E:211:TYR:O	1:E:215:LEU:HG	2.20	0.41
1:E:224:MET:HB2	1:E:225:PRO:HD3	2.03	0.41
1:F:82:VAL:CG1	2:F:302:BOG:H6'1	2.50	0.41
1:A:218:LEU:HD22	2:A:306:BOG:H7'2	2.03	0.41
1:D:213:VAL:O	1:D:219:VAL:HG11	2.21	0.41
1:B:97:PHE:CZ	1:B:123:LEU:HD21	2.56	0.41
1:C:77:LEU:HD22	1:E:70:LEU:HD21	2.02	0.41
1:D:26:VAL:O	1:D:29:PRO:HD2	2.21	0.41
1:A:44:ALA:O	1:A:48:PHE:HB2	2.21	0.40
1:A:179:ASP:HB2	1:A:192:MET:HE1	2.02	0.40
1:F:82:VAL:HG12	2:F:302:BOG:C6'	2.51	0.40
1:F:224:MET:HB2	1:F:225:PRO:HD3	2.04	0.40
1:B:172:MET:HA	1:B:175:VAL:HG22	2.03	0.40
1:F:152:SER:HA	1:F:158:ASN:HA	2.03	0.40
1:A:85:THR:O	1:A:89:ILE:HG13	2.22	0.40
2:A:302:BOG:O5	2:A:302:BOG:C2'	2.69	0.40
1:C:10:LEU:CD1	1:C:210:THR:HA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:CYS:HB3	1:C:234:PHE:CZ	2.56	0.40
1:D:17:MET:CE	1:D:229:ALA:HB2	2.52	0.40
1:F:96:PRO:HA	1:F:130:THR:HG21	2.03	0.40
2:B:302:BOG:H4'2	2:B:302:BOG:C8'	2.50	0.40
1:F:41:ILE:HD11	1:F:45:ILE:HD11	2.04	0.40
1:B:100:PHE:HE1	1:B:122:GLU:HG3	1.85	0.40
1:D:32:ILE:HD11	1:D:97:PHE:CZ	2.57	0.40
1:E:187:LEU:HD13	1:E:235:TRP:HH2	1.87	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	234/246 (95%)	226 (97%)	7 (3%)	1 (0%)	34	67
1	B	234/246 (95%)	225 (96%)	8 (3%)	1 (0%)	34	67
1	C	239/246 (97%)	227 (95%)	12 (5%)	0	100	100
1	D	238/246 (97%)	229 (96%)	9 (4%)	0	100	100
1	E	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
1	F	238/246 (97%)	229 (96%)	7 (3%)	2 (1%)	19	51
All	All	1421/1476 (96%)	1368 (96%)	49 (3%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	5	SER
1	B	116	PRO
1	F	217	PRO
1	A	217	PRO

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	198/205 (97%)	193 (98%)	5 (2%)	47	72
1	B	197/205 (96%)	190 (96%)	7 (4%)	35	63
1	C	201/205 (98%)	196 (98%)	5 (2%)	47	72
1	D	196/205 (96%)	193 (98%)	3 (2%)	65	82
1	E	196/205 (96%)	193 (98%)	3 (2%)	65	82
1	F	200/205 (98%)	197 (98%)	3 (2%)	65	82
All	All	1188/1230 (97%)	1162 (98%)	26 (2%)	52	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	8	GLN
1	F	133	ARG
1	F	218	LEU
1	A	5	SER
1	A	23	ARG
1	A	24	LEU
1	A	31	SER
1	A	166	LEU
1	B	24	LEU
1	B	26	VAL
1	B	27	LEU
1	B	112	THR
1	B	113	ASP
1	B	114	ASP
1	B	185	HIS
1	C	136	ARG
1	C	166	LEU
1	C	210	THR
1	C	211	TYR
1	C	212	LEU
1	D	4	LEU
1	D	175	VAL

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Mol	Chain	Res	Type
1	D	187	LEU
1	E	45	ILE
1	E	190	ASN
1	E	241	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	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)

20 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	F	301	-	20,20,20	1.20	2 (10%)	25,25,25	1.98	7 (28%)
2	BOG	A	306	-	20,20,20	1.18	1 (5%)	25,25,25	1.17	1 (4%)
2	BOG	E	301	-	20,20,20	1.23	2 (10%)	25,25,25	1.15	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BOG	F	304	-	20,20,20	1.17	1 (5%)	25,25,25	0.94	1 (4%)
2	BOG	A	303	-	20,20,20	1.24	2 (10%)	25,25,25	1.46	4 (16%)
2	BOG	A	301	-	20,20,20	1.16	1 (5%)	25,25,25	1.24	4 (16%)
2	BOG	A	302	-	20,20,20	1.24	2 (10%)	25,25,25	1.87	7 (28%)
2	BOG	B	302	-	20,20,20	1.10	1 (5%)	25,25,25	1.49	6 (24%)
2	BOG	F	305	-	20,20,20	1.13	2 (10%)	25,25,25	0.99	1 (4%)
2	BOG	D	302	-	20,20,20	1.38	2 (10%)	25,25,25	1.80	8 (32%)
2	BOG	F	303	-	20,20,20	1.11	1 (5%)	25,25,25	1.11	1 (4%)
2	BOG	A	304	-	20,20,20	1.10	1 (5%)	25,25,25	1.40	3 (12%)
2	BOG	F	302	-	20,20,20	1.05	1 (5%)	25,25,25	1.59	7 (28%)
2	BOG	D	301	-	20,20,20	1.20	2 (10%)	25,25,25	1.44	2 (8%)
2	BOG	C	301	-	20,20,20	1.18	2 (10%)	25,25,25	1.46	5 (20%)
2	BOG	C	303	-	20,20,20	1.25	2 (10%)	25,25,25	1.80	5 (20%)
2	BOG	B	301	-	20,20,20	1.17	1 (5%)	25,25,25	1.95	4 (16%)
2	BOG	E	302	-	20,20,20	1.18	1 (5%)	25,25,25	1.59	5 (20%)
2	BOG	C	302	-	20,20,20	1.23	1 (5%)	25,25,25	1.41	4 (16%)
2	BOG	A	305	-	20,20,20	1.24	1 (5%)	25,25,25	1.26	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
2	BOG	F	301	-	-	8/11/31/31	0/1/1/1
2	BOG	A	306	-	-	7/11/31/31	0/1/1/1
2	BOG	E	301	-	-	3/11/31/31	0/1/1/1
2	BOG	F	304	-	-	5/11/31/31	0/1/1/1
2	BOG	A	303	-	-	3/11/31/31	0/1/1/1
2	BOG	A	301	-	-	7/11/31/31	0/1/1/1
2	BOG	A	302	-	-	7/11/31/31	0/1/1/1
2	BOG	B	302	-	-	3/11/31/31	0/1/1/1
2	BOG	F	305	-	-	7/11/31/31	0/1/1/1
2	BOG	D	302	-	-	2/11/31/31	0/1/1/1
2	BOG	F	303	-	-	5/11/31/31	0/1/1/1
2	BOG	A	304	-	-	2/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	F	302	-	-	2/11/31/31	0/1/1/1
2	BOG	D	301	-	-	0/11/31/31	0/1/1/1
2	BOG	C	301	-	-	6/11/31/31	0/1/1/1
2	BOG	C	303	-	-	7/11/31/31	0/1/1/1
2	BOG	B	301	-	-	5/11/31/31	0/1/1/1
2	BOG	E	302	-	-	3/11/31/31	0/1/1/1
2	BOG	C	302	-	-	0/11/31/31	0/1/1/1
2	BOG	A	305	-	-	5/11/31/31	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	BOG	O5-C1	5.00	1.54	1.41
2	A	301	BOG	O5-C1	3.96	1.51	1.41
2	A	305	BOG	O5-C1	3.95	1.51	1.41
2	E	302	BOG	O5-C1	3.90	1.51	1.41
2	C	302	BOG	O5-C1	3.87	1.51	1.41
2	F	304	BOG	O5-C1	3.66	1.51	1.41
2	A	306	BOG	O5-C1	3.57	1.50	1.41
2	C	303	BOG	O5-C1	3.56	1.50	1.41
2	D	301	BOG	O5-C1	3.55	1.50	1.41
2	F	305	BOG	O5-C1	3.48	1.50	1.41
2	C	301	BOG	O5-C1	3.42	1.50	1.41
2	B	301	BOG	O5-C1	3.42	1.50	1.41
2	F	303	BOG	O5-C1	3.36	1.50	1.41
2	A	302	BOG	O5-C1	3.32	1.50	1.41
2	A	303	BOG	O5-C1	3.27	1.50	1.41
2	E	301	BOG	O5-C1	3.25	1.50	1.41
2	A	304	BOG	O5-C1	3.23	1.50	1.41
2	B	302	BOG	O5-C1	3.15	1.49	1.41
2	F	302	BOG	O5-C1	3.12	1.49	1.41
2	F	301	BOG	O5-C1	3.10	1.49	1.41
2	C	301	BOG	O1-C1	-2.47	1.36	1.40
2	E	301	BOG	O1-C1	-2.43	1.36	1.40
2	C	303	BOG	C3-C2	-2.38	1.46	1.52
2	F	301	BOG	O1-C1	-2.34	1.36	1.40
2	A	302	BOG	O1-C1	-2.22	1.36	1.40
2	A	303	BOG	O1-C1	-2.16	1.36	1.40
2	D	301	BOG	C3-C2	-2.04	1.47	1.52
2	D	302	BOG	O3-C3	2.03	1.47	1.43
2	F	305	BOG	O1-C1	-2.01	1.36	1.40

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	BOG	O3-C3-C4	-6.40	95.54	110.35
2	B	301	BOG	O2-C2-C1	5.29	122.89	110.05
2	B	301	BOG	C1-C2-C3	4.63	119.64	110.00
2	B	301	BOG	O1-C1-C2	4.50	115.33	108.30
2	C	303	BOG	O3-C3-C2	-4.38	100.23	110.35
2	A	302	BOG	C1-C2-C3	4.37	119.09	110.00
2	C	303	BOG	O2-C2-C3	-4.26	100.50	110.35
2	A	302	BOG	O2-C2-C1	4.16	120.14	110.05
2	E	302	BOG	O1-C1-C2	3.84	114.31	108.30
2	F	301	BOG	C4-C3-C2	3.71	117.31	110.82
2	A	302	BOG	O2-C2-C3	3.56	118.58	110.35
2	A	304	BOG	O1-C1-C2	3.54	113.83	108.30
2	F	302	BOG	O1-C1-C2	3.44	113.67	108.30
2	E	301	BOG	O1-C1-C2	3.41	113.62	108.30
2	C	302	BOG	O5-C5-C6	3.39	114.87	106.44
2	A	305	BOG	O5-C5-C6	3.37	114.83	106.44
2	D	301	BOG	C1-O5-C5	-3.36	107.10	113.69
2	F	302	BOG	C1-O5-C5	-3.31	107.19	113.69
2	C	302	BOG	C1-O5-C5	-3.30	107.20	113.69
2	C	303	BOG	O3-C3-C4	3.30	117.99	110.35
2	D	302	BOG	O5-C1-C2	3.27	117.26	110.35
2	A	306	BOG	O2-C2-C3	-3.24	102.85	110.35
2	D	302	BOG	C3'-C2'-C1'	-3.20	99.30	113.49
2	A	303	BOG	C6-C5-C4	-3.13	105.67	113.00
2	E	301	BOG	C1-O5-C5	-3.12	107.57	113.69
2	B	302	BOG	C1-O5-C5	-3.10	107.60	113.69
2	B	302	BOG	O1-C1-C2	3.06	113.08	108.30
2	A	304	BOG	O4-C4-C5	-3.03	101.76	109.30
2	D	302	BOG	C6'-C5'-C4'	-2.98	99.31	114.42
2	D	302	BOG	O1-C1-C2	-2.93	103.73	108.30
2	C	303	BOG	O2-C2-C1	2.91	117.12	110.05
2	C	301	BOG	C3-C4-C5	2.87	115.36	110.24
2	A	303	BOG	C4-C3-C2	-2.83	105.88	110.82
2	A	301	BOG	C1'-O1-C1	2.83	118.53	113.84
2	A	302	BOG	C1-O5-C5	-2.81	108.18	113.69
2	F	304	BOG	O1-C1-C2	2.79	112.66	108.30
2	D	301	BOG	O3-C3-C2	-2.72	104.06	110.35
2	E	302	BOG	C1-O5-C5	-2.72	108.36	113.69
2	F	301	BOG	C1'-O1-C1	2.61	118.16	113.84
2	C	301	BOG	O5-C1-C2	2.57	115.79	110.35
2	E	302	BOG	O5-C1-C2	-2.55	104.94	110.35
2	C	301	BOG	O5-C5-C4	2.54	114.31	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	BOG	C6-C5-C4	-2.52	107.11	113.00
2	A	303	BOG	O5-C5-C4	2.48	114.20	109.69
2	A	303	BOG	C3-C4-C5	-2.47	105.84	110.24
2	F	302	BOG	O5-C1-O1	-2.46	104.14	109.97
2	F	302	BOG	O4-C4-C3	2.46	116.04	110.35
2	A	301	BOG	O1-C1-C2	2.43	112.09	108.30
2	B	302	BOG	C6-C5-C4	-2.43	107.32	113.00
2	F	301	BOG	O4-C4-C5	2.41	115.28	109.30
2	A	302	BOG	O4-C4-C3	-2.37	104.87	110.35
2	A	302	BOG	O3-C3-C4	-2.36	104.90	110.35
2	E	302	BOG	O5-C1-O1	2.35	115.54	109.97
2	D	302	BOG	O5-C5-C4	2.32	113.91	109.69
2	F	305	BOG	C4-C3-C2	2.31	114.85	110.82
2	F	302	BOG	C4'-C3'-C2'	-2.30	102.77	114.42
2	C	301	BOG	C6-C5-C4	-2.30	107.63	113.00
2	B	302	BOG	O6-C6-C5	-2.29	103.42	111.29
2	B	302	BOG	O4-C4-C5	-2.29	103.61	109.30
2	A	301	BOG	O5-C5-C6	2.25	112.03	106.44
2	A	302	BOG	O1-C1-C2	2.24	111.81	108.30
2	E	302	BOG	O5-C5-C6	2.23	111.97	106.44
2	D	302	BOG	C1-O5-C5	2.22	118.04	113.69
2	F	302	BOG	C1'-O1-C1	2.22	117.51	113.84
2	D	302	BOG	C5'-C4'-C3'	-2.19	103.31	114.42
2	A	304	BOG	O5-C5-C4	2.19	113.67	109.69
2	F	301	BOG	C1-O5-C5	-2.19	109.39	113.69
2	B	301	BOG	O2-C2-C3	2.13	115.27	110.35
2	C	302	BOG	O2-C2-C1	2.13	115.22	110.05
2	C	302	BOG	C1'-O1-C1	2.13	117.37	113.84
2	F	303	BOG	C1-O5-C5	-2.09	109.58	113.69
2	F	301	BOG	O5-C1-O1	-2.08	105.05	109.97
2	F	301	BOG	C6-C5-C4	-2.08	108.13	113.00
2	C	301	BOG	O1-C1-C2	-2.06	105.08	108.30
2	C	303	BOG	C1-O5-C5	-2.05	109.66	113.69
2	F	302	BOG	O4-C4-C5	-2.03	104.25	109.30
2	B	302	BOG	O5-C5-C4	2.03	113.38	109.69
2	D	302	BOG	C3-C4-C5	2.02	113.83	110.24

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	BOG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
2	F	303	BOG	C2'-C1'-O1-C1
2	F	304	BOG	O5-C1-O1-C1'
2	F	304	BOG	C2'-C1'-O1-C1
2	A	301	BOG	C2'-C1'-O1-C1
2	B	301	BOG	C2-C1-O1-C1'
2	B	301	BOG	O5-C1-O1-C1'
2	E	302	BOG	C2'-C1'-O1-C1
2	F	301	BOG	C4-C5-C6-O6
2	F	301	BOG	O5-C5-C6-O6
2	F	304	BOG	C4-C5-C6-O6
2	A	306	BOG	O5-C1-O1-C1'
2	F	301	BOG	C2-C1-O1-C1'
2	A	301	BOG	C3'-C4'-C5'-C6'
2	F	304	BOG	O5-C5-C6-O6
2	C	301	BOG	O5-C5-C6-O6
2	D	302	BOG	O5-C5-C6-O6
2	A	304	BOG	O1-C1'-C2'-C3'
2	F	303	BOG	O5-C1-O1-C1'
2	E	301	BOG	O5-C1-O1-C1'
2	C	303	BOG	O5-C5-C6-O6
2	A	306	BOG	C4-C5-C6-O6
2	B	301	BOG	O5-C5-C6-O6
2	E	301	BOG	C2'-C3'-C4'-C5'
2	B	301	BOG	O1-C1'-C2'-C3'
2	F	303	BOG	C2-C1-O1-C1'
2	F	305	BOG	C4'-C5'-C6'-C7'
2	B	301	BOG	C2'-C3'-C4'-C5'
2	A	302	BOG	C3'-C4'-C5'-C6'
2	A	305	BOG	C4'-C5'-C6'-C7'
2	A	305	BOG	C2'-C3'-C4'-C5'
2	A	306	BOG	C3'-C4'-C5'-C6'
2	A	302	BOG	C2'-C3'-C4'-C5'
2	F	304	BOG	C1'-C2'-C3'-C4'
2	A	305	BOG	C2'-C1'-O1-C1
2	C	303	BOG	C2'-C3'-C4'-C5'
2	C	303	BOG	C3'-C4'-C5'-C6'
2	A	301	BOG	C1'-C2'-C3'-C4'
2	F	305	BOG	C3'-C4'-C5'-C6'
2	F	301	BOG	C3'-C4'-C5'-C6'
2	A	306	BOG	O5-C5-C6-O6
2	A	306	BOG	C5'-C6'-C7'-C8'
2	F	301	BOG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
2	A	305	BOG	O1-C1'-C2'-C3'
2	F	305	BOG	C2-C1-O1-C1'
2	F	302	BOG	C3'-C4'-C5'-C6'
2	A	301	BOG	O1-C1'-C2'-C3'
2	F	301	BOG	O1-C1'-C2'-C3'
2	C	301	BOG	C4'-C5'-C6'-C7'
2	C	303	BOG	C4'-C5'-C6'-C7'
2	F	305	BOG	C5'-C6'-C7'-C8'
2	F	301	BOG	C5'-C6'-C7'-C8'
2	A	302	BOG	C4'-C5'-C6'-C7'
2	C	301	BOG	C2'-C3'-C4'-C5'
2	A	306	BOG	O1-C1'-C2'-C3'
2	A	303	BOG	O5-C5-C6-O6
2	C	303	BOG	C1'-C2'-C3'-C4'
2	C	303	BOG	C5'-C6'-C7'-C8'
2	B	302	BOG	C4'-C5'-C6'-C7'
2	C	301	BOG	C4-C5-C6-O6
2	A	302	BOG	C2-C1-O1-C1'
2	A	302	BOG	C1'-C2'-C3'-C4'
2	B	302	BOG	O5-C5-C6-O6
2	F	305	BOG	C2'-C1'-O1-C1
2	A	302	BOG	C2'-C1'-O1-C1
2	A	302	BOG	O1-C1'-C2'-C3'
2	A	306	BOG	C2'-C3'-C4'-C5'
2	A	301	BOG	C5'-C6'-C7'-C8'
2	F	305	BOG	O5-C1-O1-C1'
2	C	301	BOG	C5'-C6'-C7'-C8'
2	F	303	BOG	O5-C5-C6-O6
2	E	302	BOG	C4'-C5'-C6'-C7'
2	F	303	BOG	C5'-C6'-C7'-C8'
2	F	302	BOG	C5'-C6'-C7'-C8'
2	F	305	BOG	C4-C5-C6-O6
2	A	303	BOG	C2'-C3'-C4'-C5'
2	A	301	BOG	O5-C5-C6-O6
2	B	302	BOG	C2'-C3'-C4'-C5'
2	E	301	BOG	C3'-C4'-C5'-C6'
2	C	301	BOG	C3'-C4'-C5'-C6'
2	A	305	BOG	C2-C1-O1-C1'
2	E	302	BOG	C1'-C2'-C3'-C4'
2	A	301	BOG	C4'-C5'-C6'-C7'
2	D	302	BOG	C4-C5-C6-O6
2	C	303	BOG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	304	BOG	C2'-C1'-O1-C1
2	A	303	BOG	O5-C1-O1-C1'

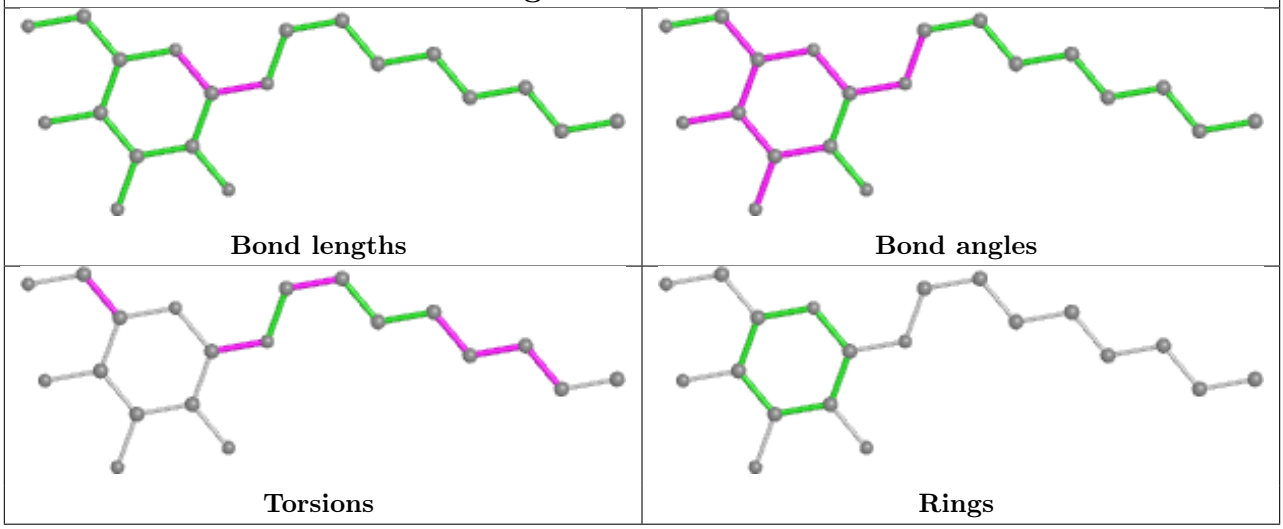
There are no ring outliers.

14 monomers are involved in 33 short contacts:

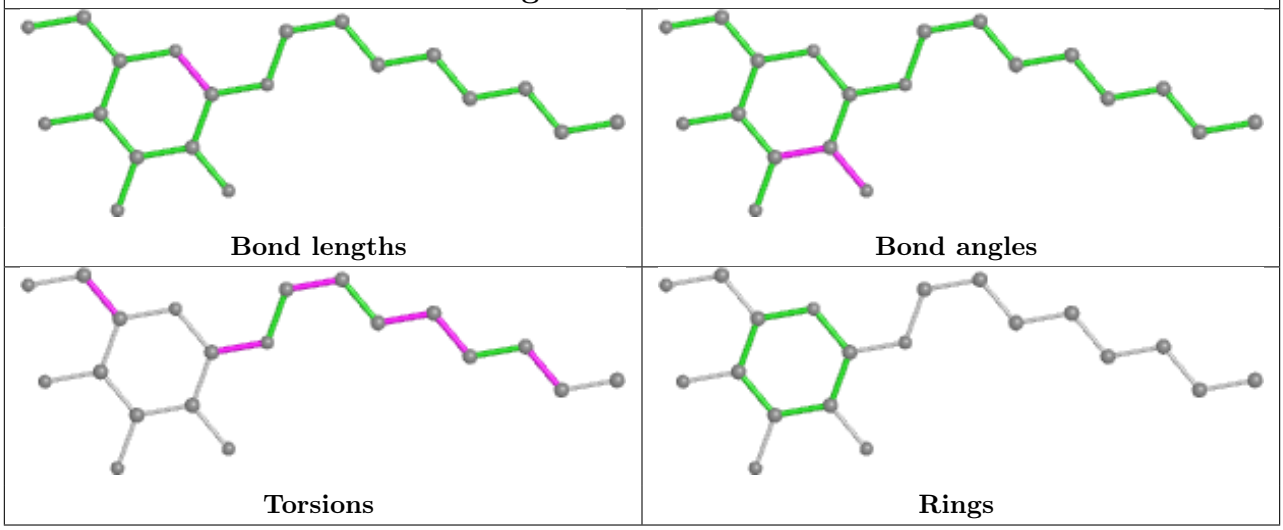
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	BOG	1	0
2	A	306	BOG	1	0
2	E	301	BOG	3	0
2	A	303	BOG	2	0
2	A	301	BOG	1	0
2	A	302	BOG	4	0
2	B	302	BOG	5	0
2	D	302	BOG	1	0
2	A	304	BOG	1	0
2	F	302	BOG	6	0
2	D	301	BOG	3	0
2	C	301	BOG	2	0
2	B	301	BOG	1	0
2	A	305	BOG	3	0

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.

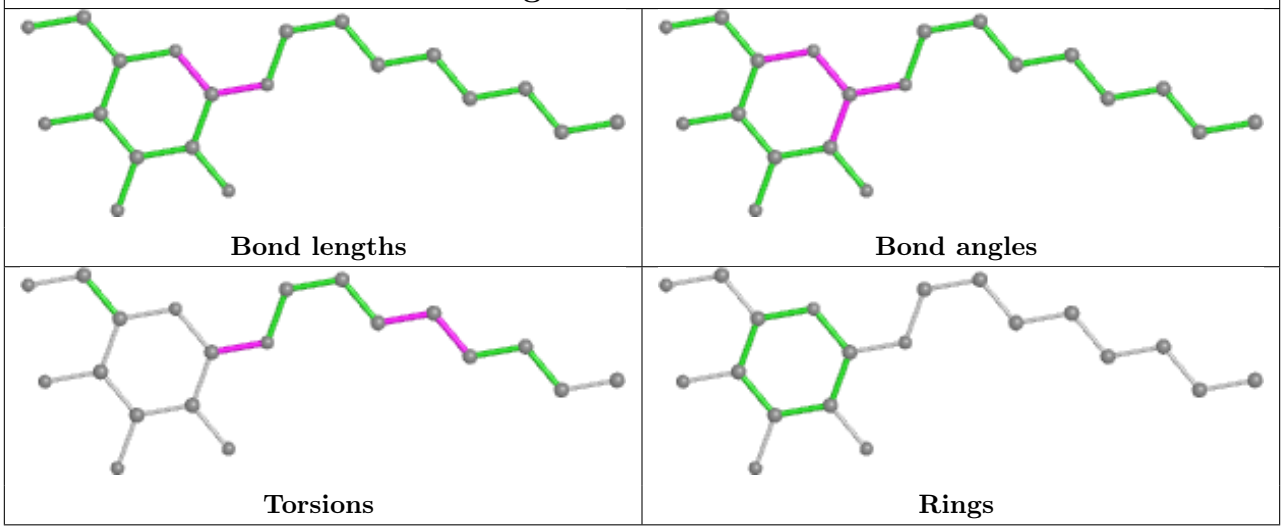
Ligand BOG F 301



Ligand BOG A 306



Ligand BOG E 301



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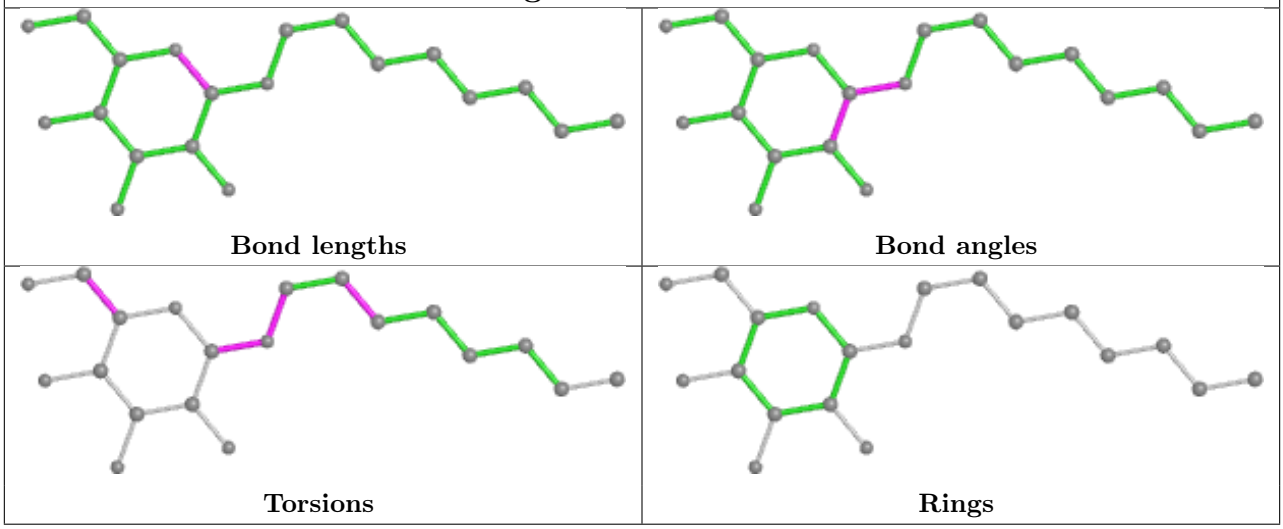

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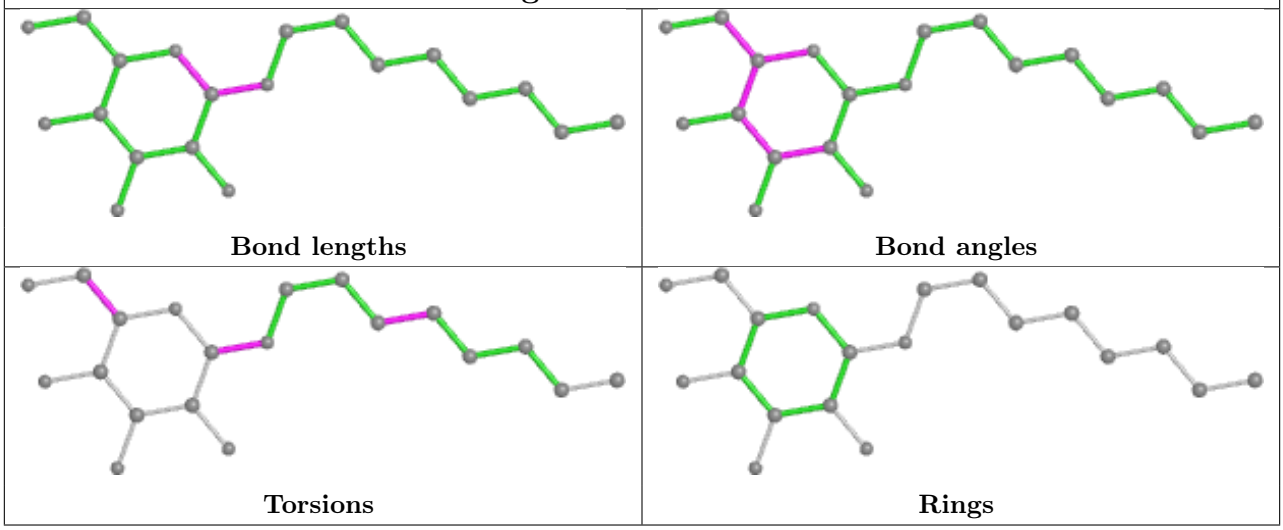

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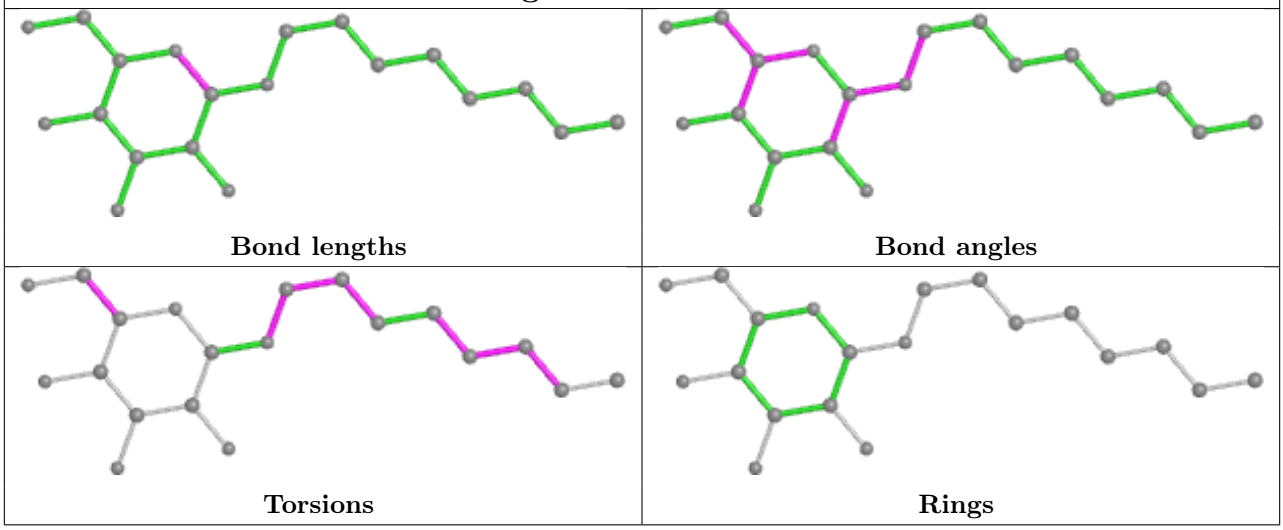

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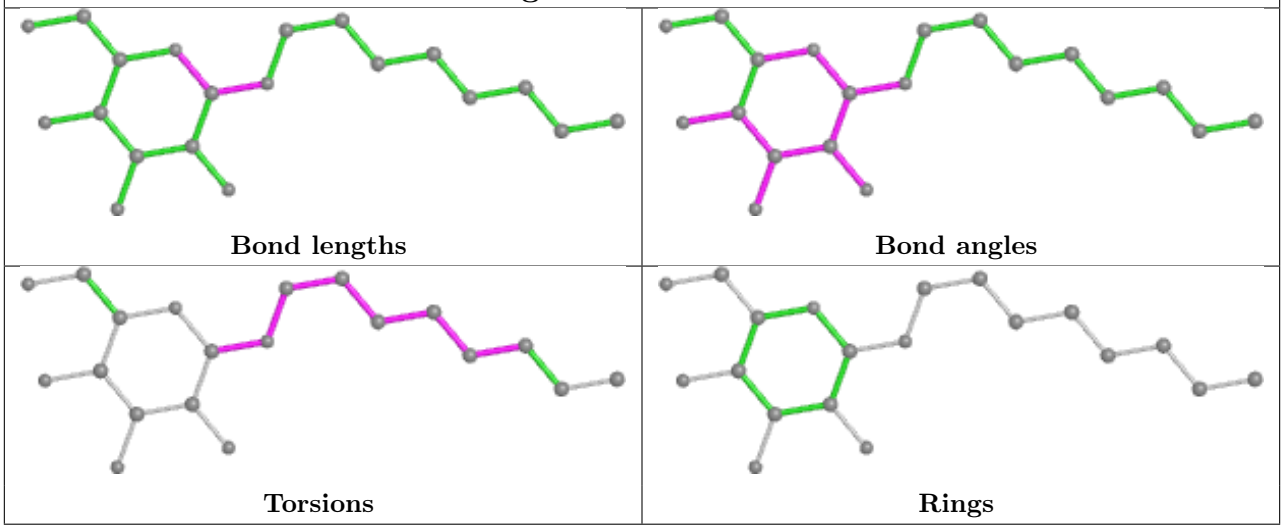
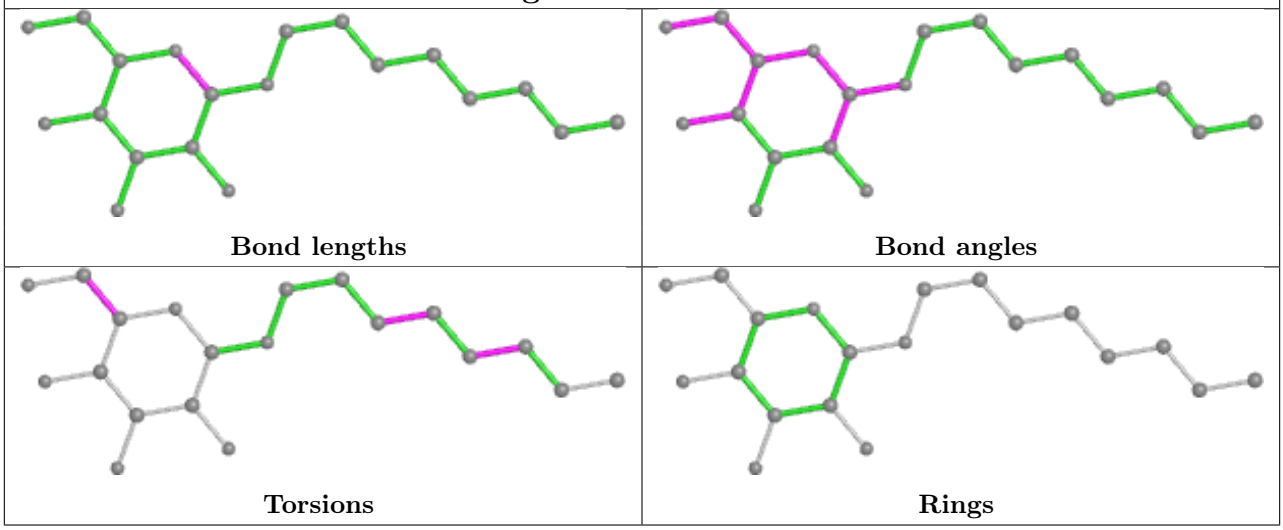


Ligand BOG B 302



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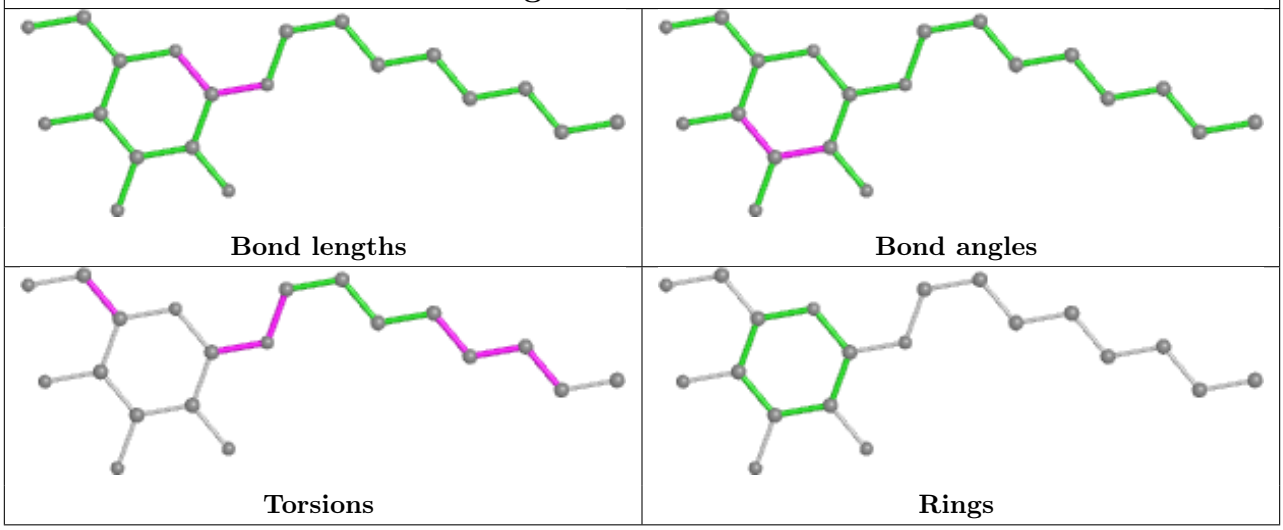
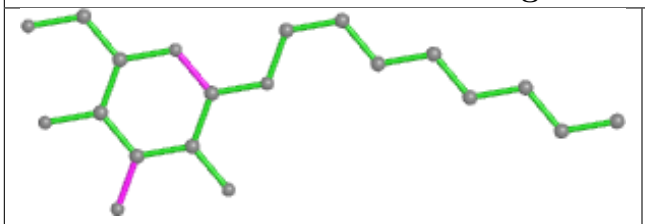
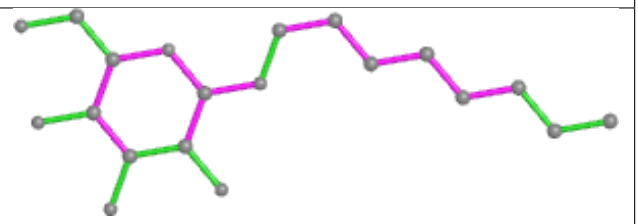


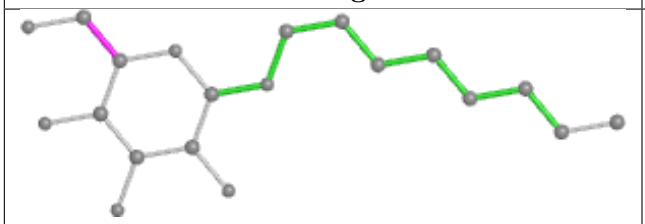
Ligand BOG D 302



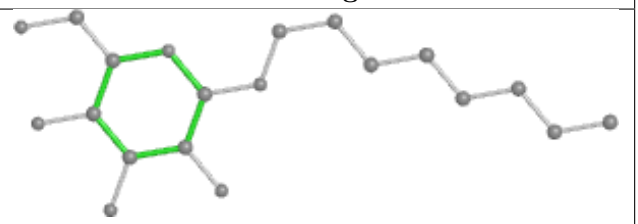
Bond lengths



Bond angles

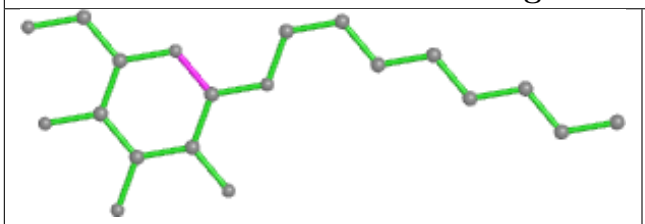


Torsions

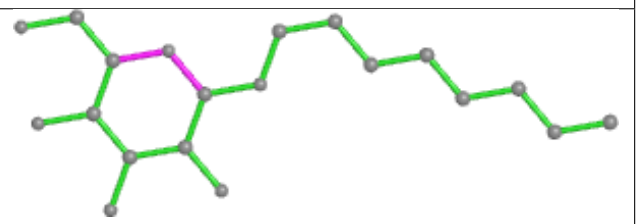


Rings

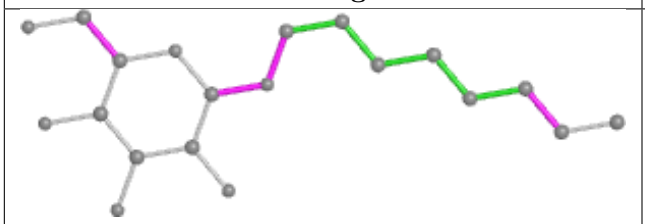
Ligand BOG F 303



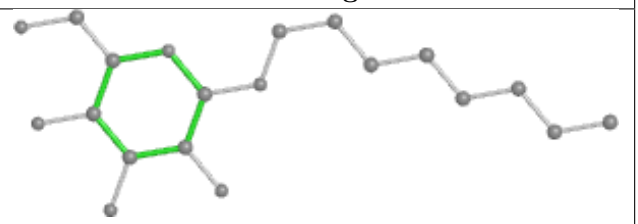
Bond lengths



Bond angles

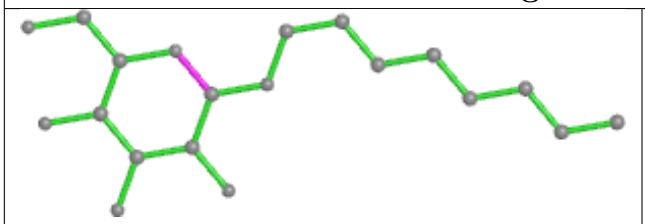


Torsions

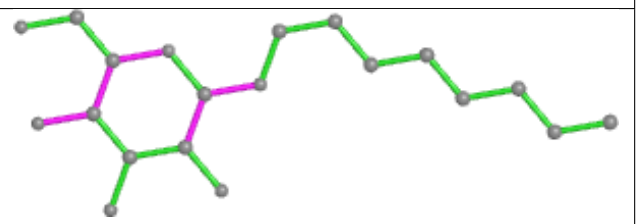


Rings

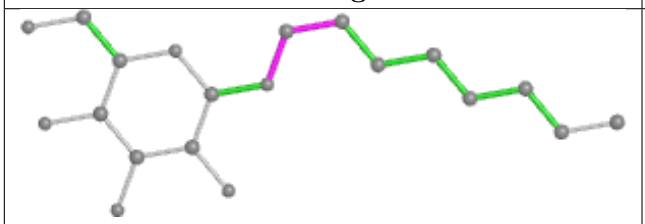
Ligand BOG A 304



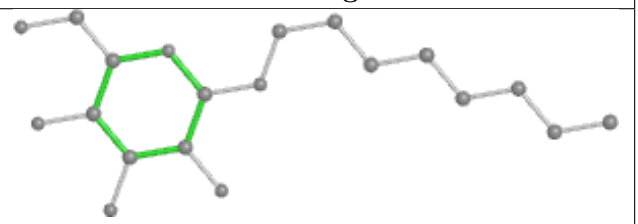
Bond lengths



Bond angles

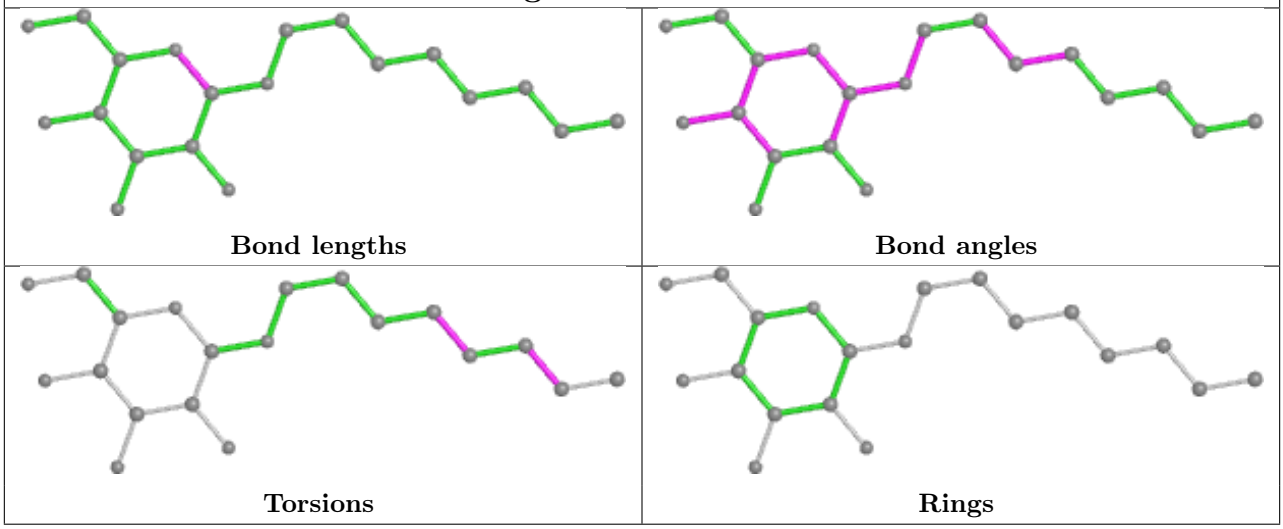


Torsions

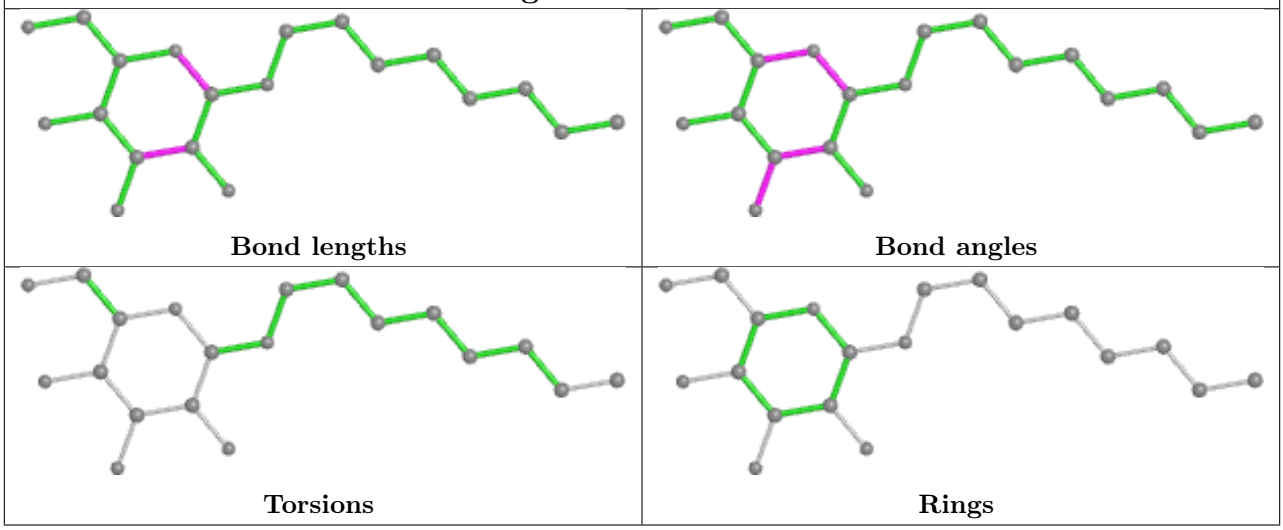


Rings

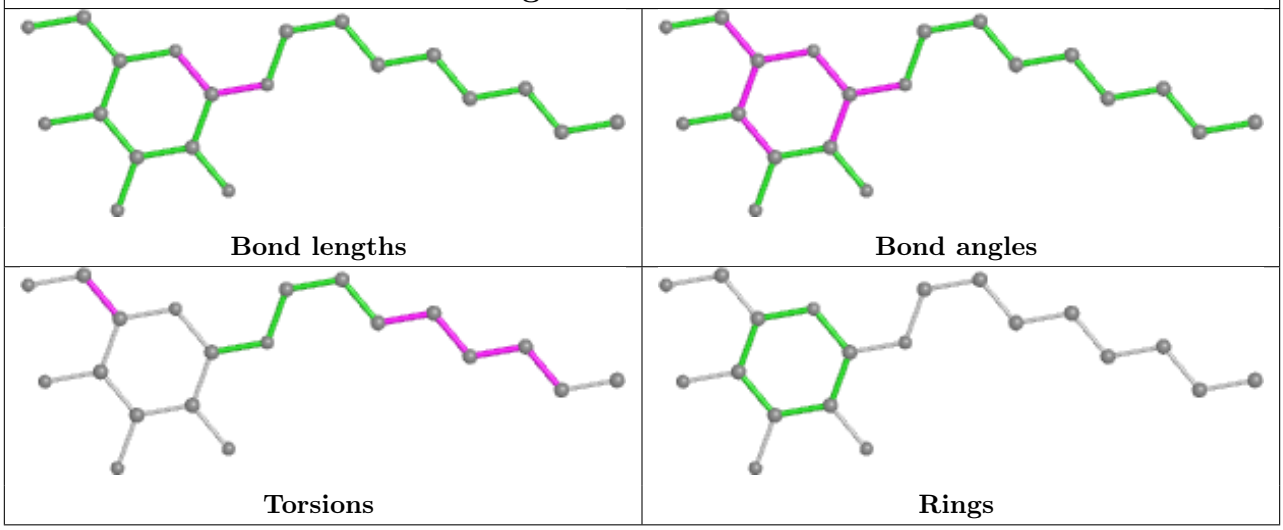
Ligand BOG F 302



Ligand BOG D 301



Ligand BOG C 301



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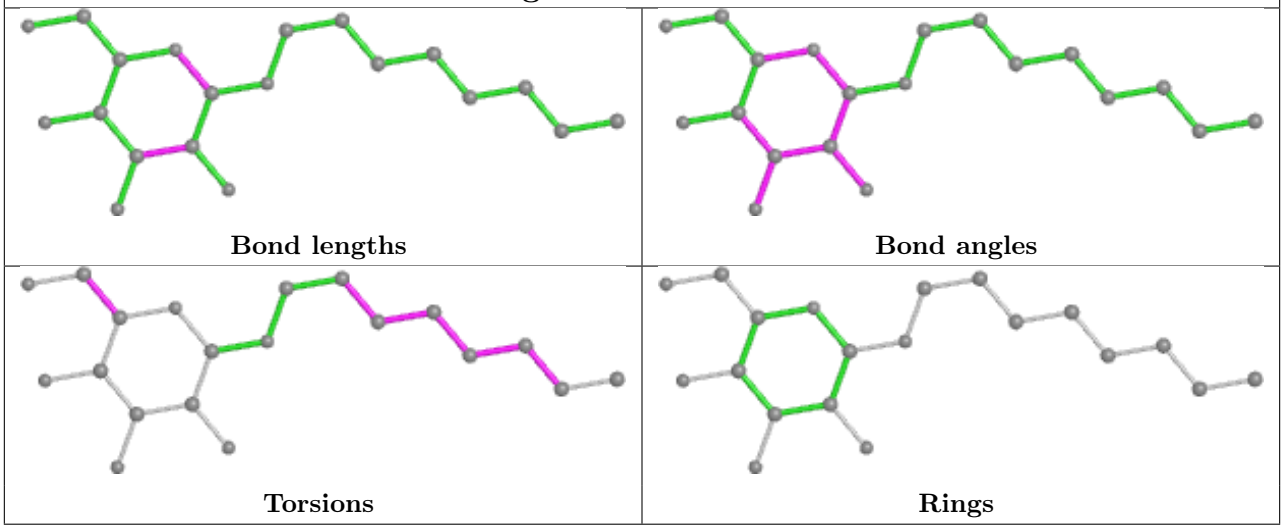
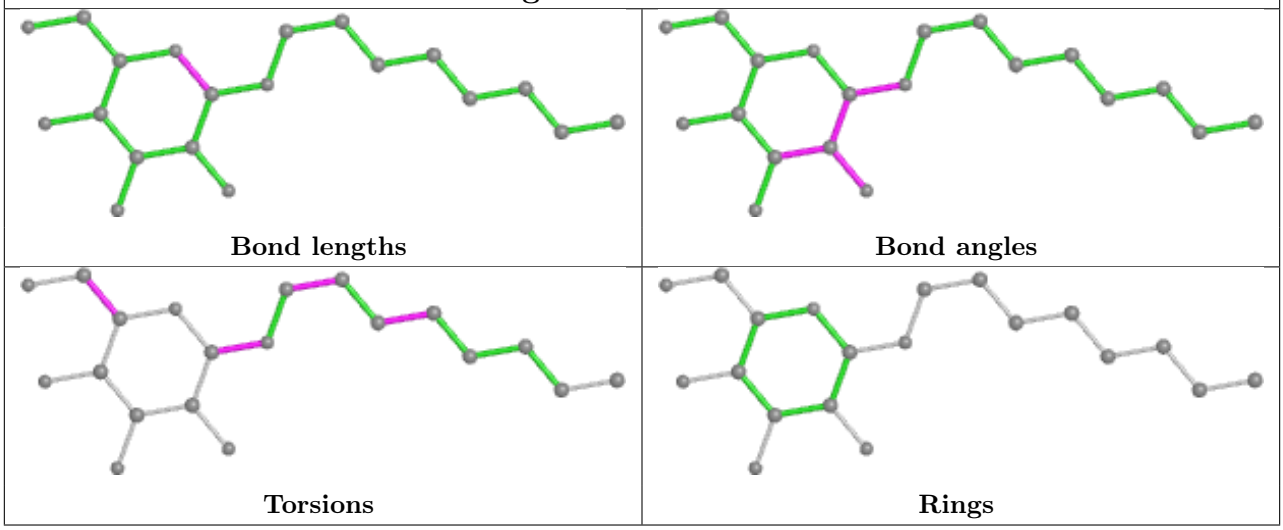
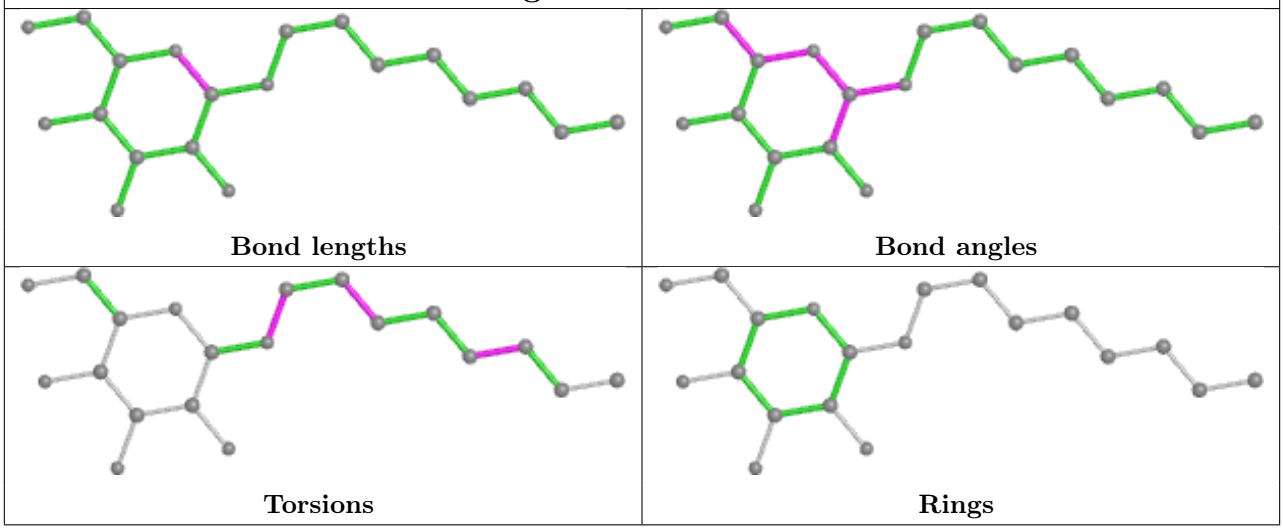


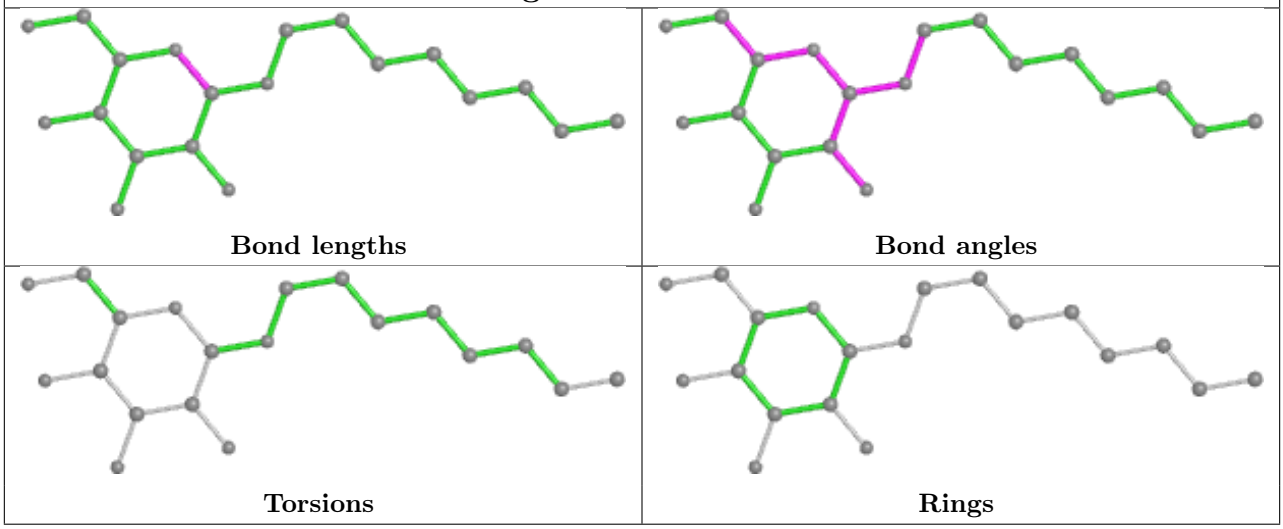
Ligand BOG B 301



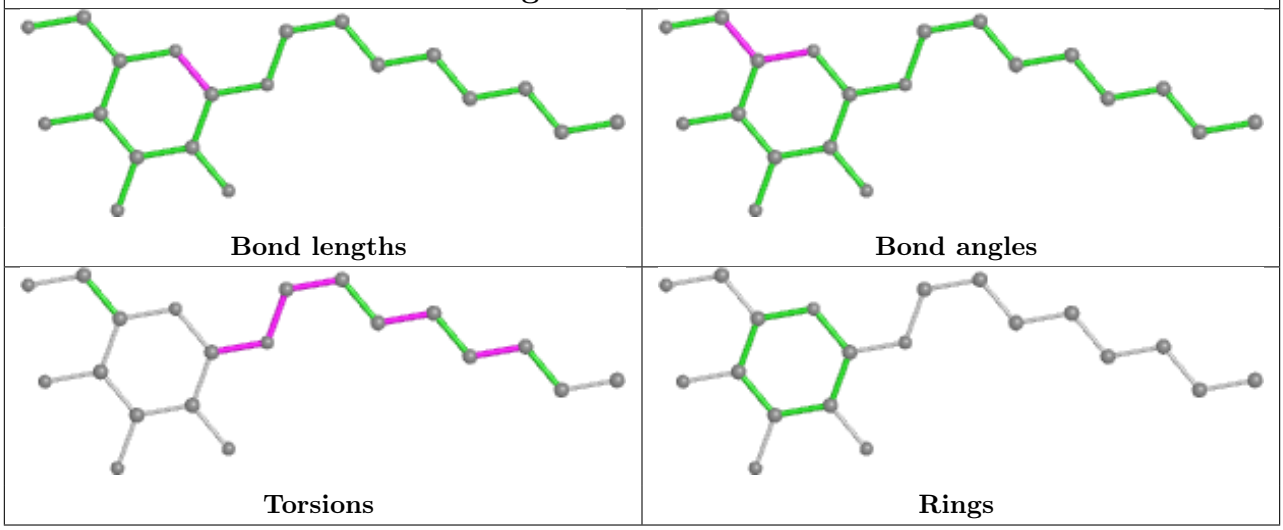
Ligand BOG E 302



Ligand BOG C 302



Ligand BOG A 305



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	236/246 (95%)	0.29	15 (6%)	19	20	132, 167, 209, 295	0
1	B	236/246 (95%)	0.88	49 (20%)	1	1	136, 209, 300, 392	0
1	C	241/246 (97%)	0.44	18 (7%)	14	16	133, 156, 209, 275	0
1	D	240/246 (97%)	0.84	38 (15%)	2	2	138, 186, 247, 299	0
1	E	240/246 (97%)	0.41	13 (5%)	25	26	141, 169, 221, 268	0
1	F	240/246 (97%)	0.43	15 (6%)	20	21	126, 155, 206, 233	0
All	All	1433/1476 (97%)	0.55	148 (10%)	6	8	126, 171, 251, 392	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	PRO	13.6
1	B	25	PHE	10.3
1	B	26	VAL	10.2
1	B	115	PHE	9.8
1	D	22	LEU	8.9
1	D	114	ASP	8.8
1	D	21	GLY	8.7
1	D	118	PHE	8.4
1	D	20	PRO	8.0
1	B	191	GLU	7.9
1	B	22	LEU	7.0
1	F	116	PRO	6.9
1	D	116	PRO	6.5
1	B	114	ASP	6.3
1	F	114	ASP	6.0
1	F	22	LEU	5.8
1	B	105	VAL	5.8
1	F	3	THR	5.6
1	D	3	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	LYS	5.4
1	B	117	ALA	5.4
1	B	27	LEU	5.4
1	D	25	PHE	5.3
1	D	5	SER	5.3
1	B	118	PHE	5.2
1	D	112	THR	5.2
1	D	218	LEU	5.0
1	D	24	LEU	4.8
1	B	24	LEU	4.7
1	F	242	GLN	4.6
1	D	115	PHE	4.6
1	D	19	ARG	4.6
1	A	237	ARG	4.3
1	B	189	TRP	4.3
1	E	118	PHE	4.2
1	E	22	LEU	4.2
1	D	28	LEU	4.1
1	C	242	GLN	4.0
1	B	222	VAL	4.0
1	B	233	LEU	3.9
1	E	218	LEU	3.9
1	B	112	THR	3.9
1	A	5	SER	3.8
1	B	107	VAL	3.8
1	D	7	PRO	3.8
1	A	62	TRP	3.7
1	E	5	SER	3.7
1	C	59	LEU	3.7
1	F	112	THR	3.6
1	F	4	LEU	3.6
1	B	113	ASP	3.6
1	C	62	TRP	3.5
1	D	113	ASP	3.5
1	F	113	ASP	3.5
1	F	62	TRP	3.5
1	B	30	LEU	3.5
1	B	19	ARG	3.5
1	B	123	LEU	3.5
1	F	118	PHE	3.5
1	B	187	LEU	3.4
1	B	232	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	6	GLY	3.4
1	D	4	LEU	3.4
1	A	236	VAL	3.3
1	B	4	LEU	3.3
1	A	141	PHE	3.3
1	D	109	VAL	3.3
1	C	186	LYS	3.3
1	B	20	PRO	3.2
1	B	21	GLY	3.2
1	A	196	LEU	3.1
1	F	25	PHE	3.1
1	B	17	MET	3.1
1	F	117	ALA	3.0
1	A	4	LEU	3.0
1	E	25	PHE	3.0
1	D	203	CYS	2.9
1	C	166	LEU	2.9
1	C	218	LEU	2.9
1	B	235	TRP	2.8
1	A	234	PHE	2.8
1	C	157	LEU	2.8
1	B	195	TRP	2.8
1	B	225	PRO	2.7
1	B	221	LEU	2.7
1	B	104	LYS	2.7
1	B	138	LEU	2.7
1	C	120	TRP	2.7
1	C	22	LEU	2.7
1	A	238	GLU	2.6
1	F	48	PHE	2.6
1	C	148	LEU	2.6
1	E	123	LEU	2.6
1	B	218	LEU	2.5
1	C	65	PHE	2.5
1	D	67	GLN	2.5
1	C	123	LEU	2.5
1	B	192	MET	2.5
1	B	5	SER	2.5
1	F	222	VAL	2.5
1	D	108	VAL	2.5
1	D	220	ASN	2.5
1	D	100	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	109	VAL	2.4
1	B	101	LEU	2.4
1	A	213	VAL	2.4
1	D	119	SER	2.4
1	D	63	LEU	2.4
1	A	233	LEU	2.4
1	D	217	PRO	2.3
1	B	127	VAL	2.3
1	C	4	LEU	2.3
1	A	235	TRP	2.3
1	D	107	VAL	2.3
1	D	97	PHE	2.3
1	B	193	LEU	2.2
1	D	37	PHE	2.2
1	A	6	GLY	2.2
1	D	150	ILE	2.2
1	E	104	LYS	2.2
1	D	196	LEU	2.2
1	D	175	VAL	2.2
1	F	218	LEU	2.2
1	A	195	TRP	2.1
1	C	16	LEU	2.1
1	A	185	HIS	2.1
1	B	142	LEU	2.1
1	B	145	ALA	2.1
1	B	190	ASN	2.1
1	B	93	ILE	2.1
1	D	212	LEU	2.1
1	E	229	ALA	2.1
1	C	232	VAL	2.1
1	B	188	GLY	2.1
1	C	66	LEU	2.1
1	C	63	LEU	2.1
1	D	104	LYS	2.1
1	E	119	SER	2.1
1	B	16	LEU	2.1
1	C	118	PHE	2.1
1	D	59	LEU	2.1
1	E	124	MET	2.1
1	E	108	VAL	2.1
1	B	236	VAL	2.0
1	D	27	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	157	LEU	2.0
1	E	16	LEU	2.0
1	B	129	ARG	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)

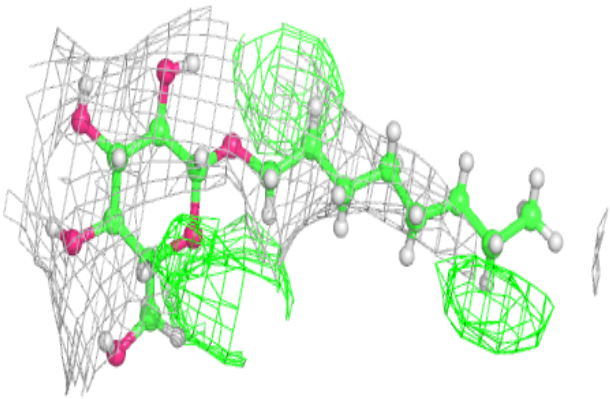
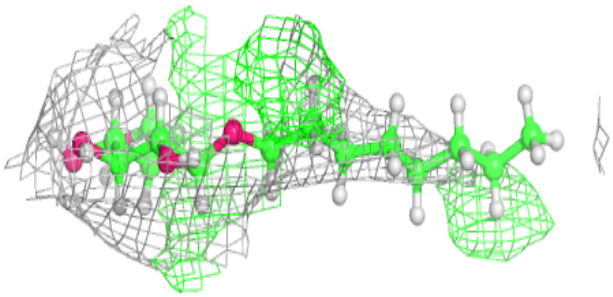
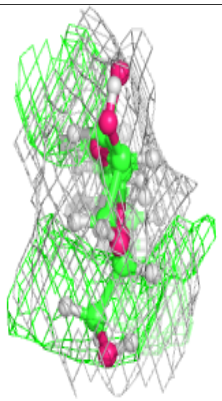
There are no monosaccharides in this entry.

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.

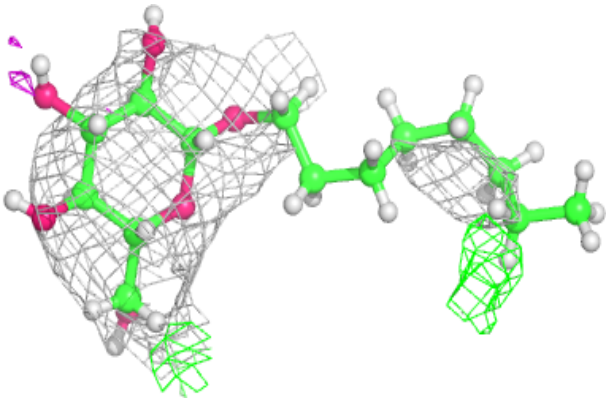
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BOG	D	302	20/20	0.49	0.40	160,192,202,203	0
2	BOG	F	305	20/20	0.58	0.54	160,193,201,202	0
2	BOG	E	301	20/20	0.62	0.48	159,198,201,202	0
2	BOG	A	305	20/20	0.69	0.76	159,194,199,202	0
2	BOG	F	304	20/20	0.70	0.39	161,193,200,201	0
2	BOG	C	302	20/20	0.72	0.45	161,194,198,201	0
2	BOG	C	303	20/20	0.75	0.59	161,194,199,202	0
2	BOG	A	302	20/20	0.76	0.36	160,194,201,201	0
2	BOG	F	301	20/20	0.77	0.55	159,191,199,199	0
2	BOG	B	302	20/20	0.79	0.65	164,198,200,202	0
2	BOG	E	302	20/20	0.79	0.54	160,194,198,200	0
2	BOG	F	302	20/20	0.80	0.52	161,193,199,201	0
2	BOG	B	301	20/20	0.80	0.85	162,196,200,201	0
2	BOG	A	306	20/20	0.82	0.60	159,194,198,199	0
2	BOG	D	301	20/20	0.83	0.36	159,191,200,202	0
2	BOG	A	303	20/20	0.83	0.57	162,194,199,200	0
2	BOG	C	301	20/20	0.84	0.90	163,195,199,201	0
2	BOG	A	301	20/20	0.85	0.36	160,193,197,199	0
2	BOG	F	303	20/20	0.85	0.32	161,193,198,198	0
2	BOG	A	304	20/20	0.87	0.30	160,193,197,199	0

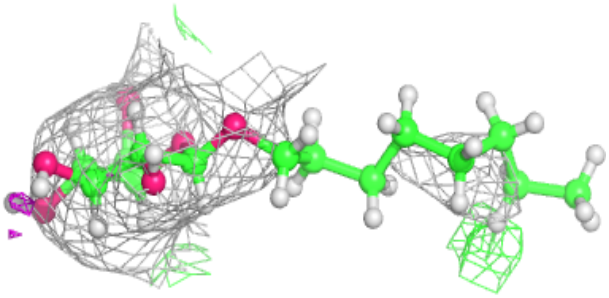
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

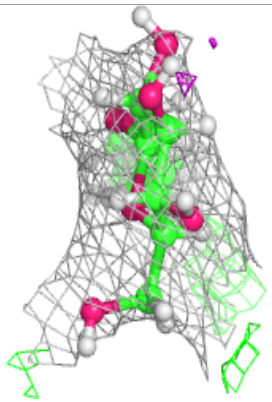
Electron density around BOG D 302: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around BOG F 305:

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

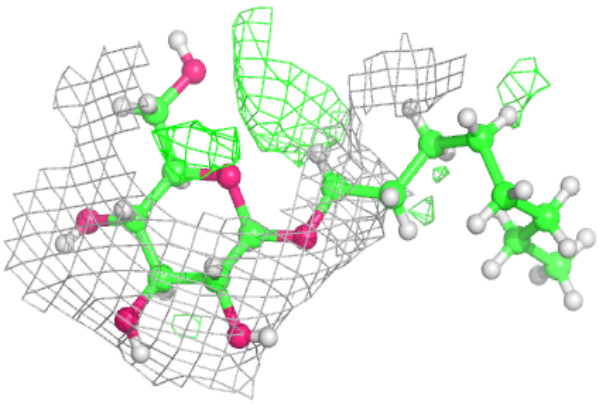


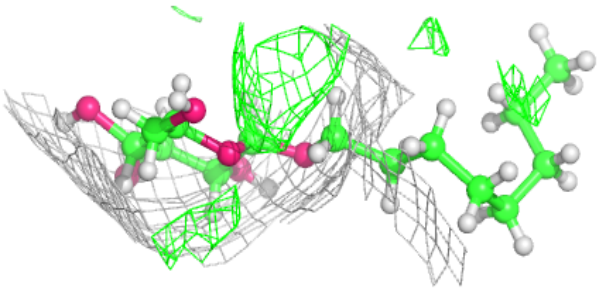


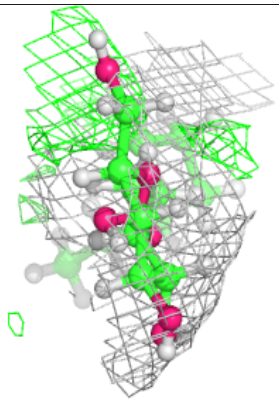


Electron density around BOG E 301:

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

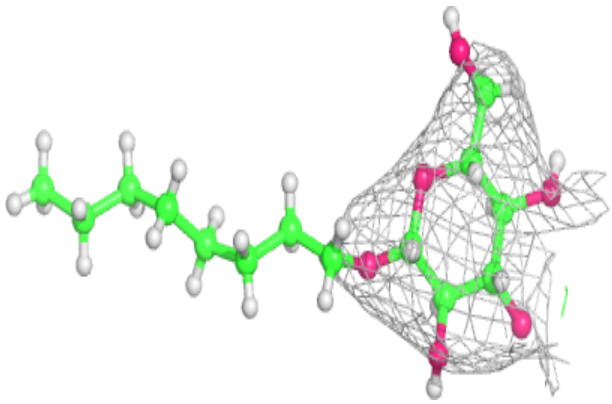


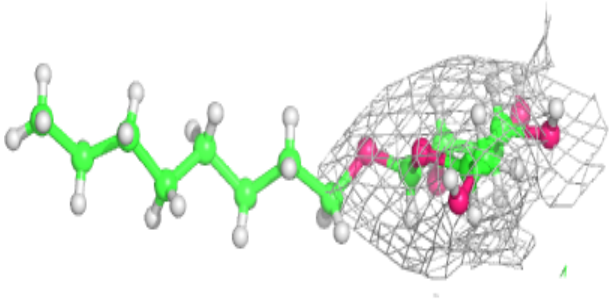


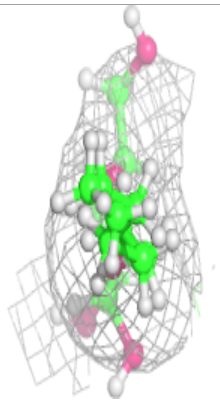


Electron density around BOG A 305:

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

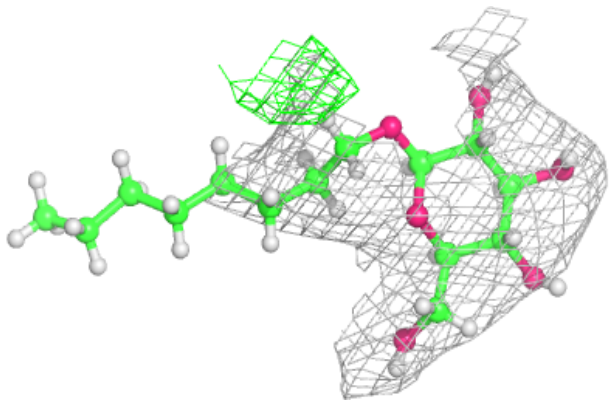


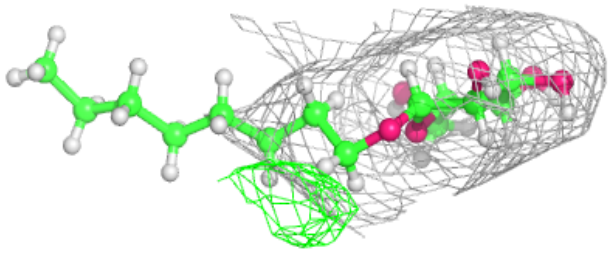


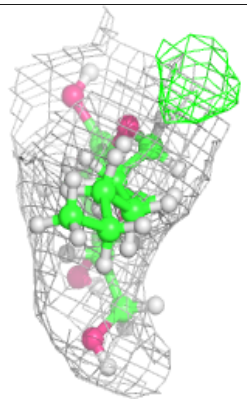


Electron density around BOG F 304:

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

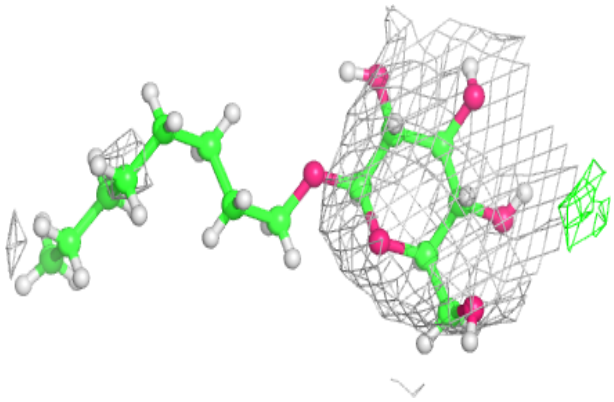


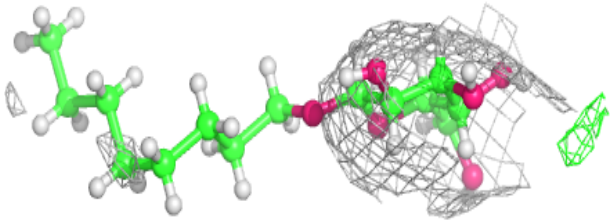


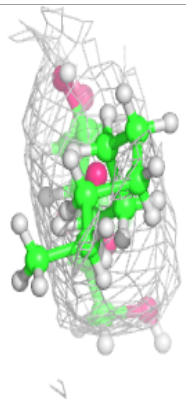


Electron density around BOG C 302:

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

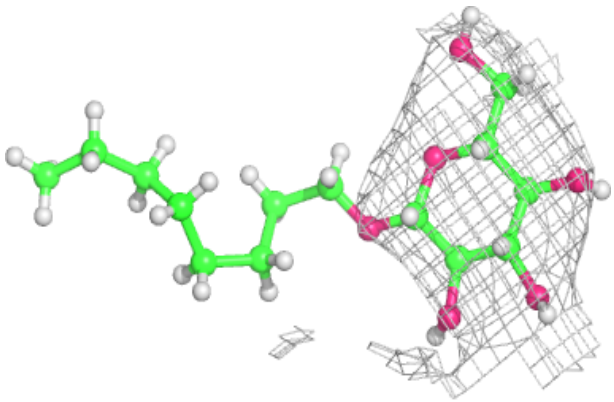


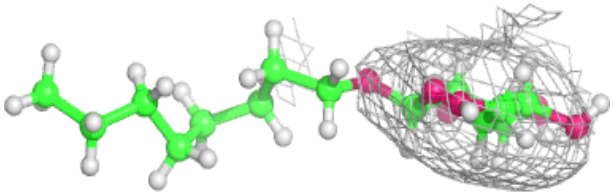


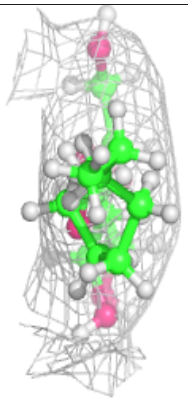


Electron density around BOG C 303:

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

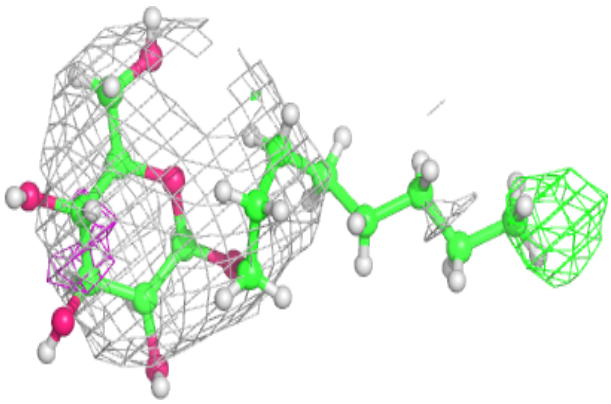


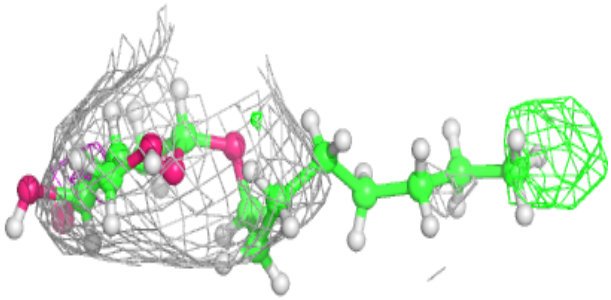


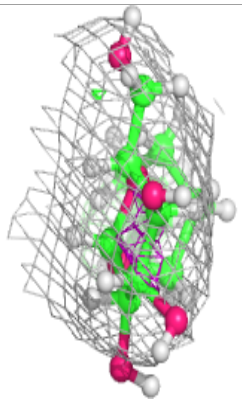


Electron density around BOG A 302:

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

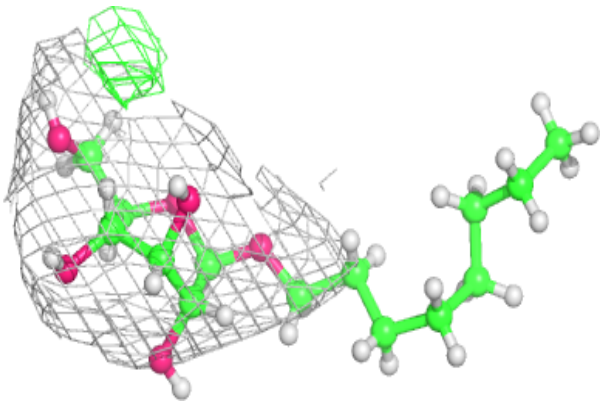


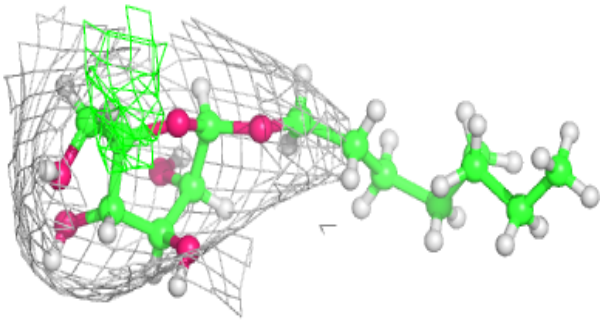


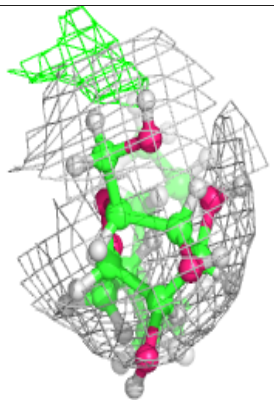


Electron density around BOG F 301:

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

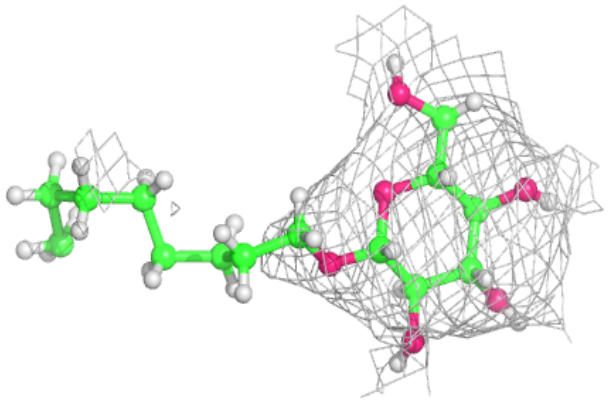


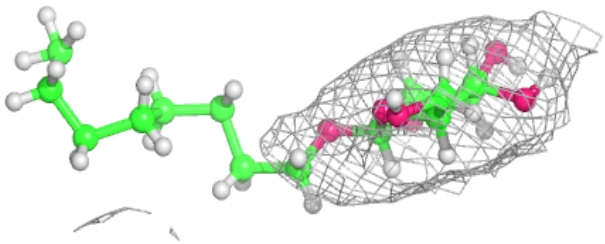


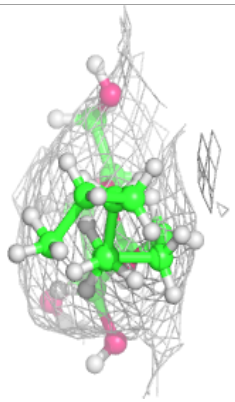


Electron density around BOG B 302:

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

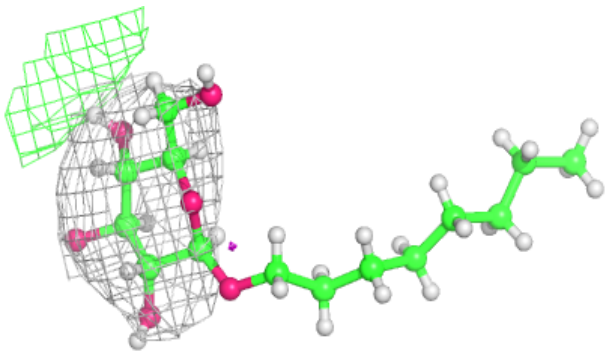


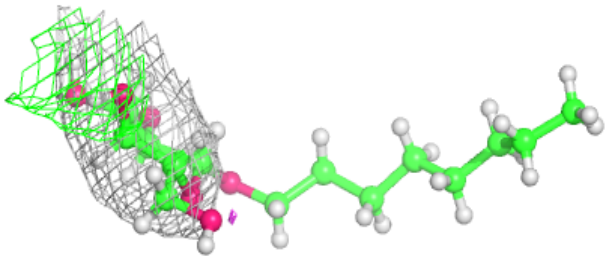


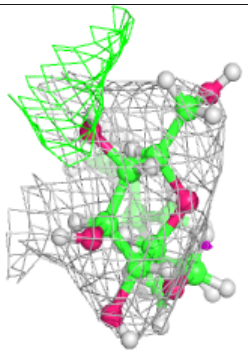


Electron density around BOG E 302:

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

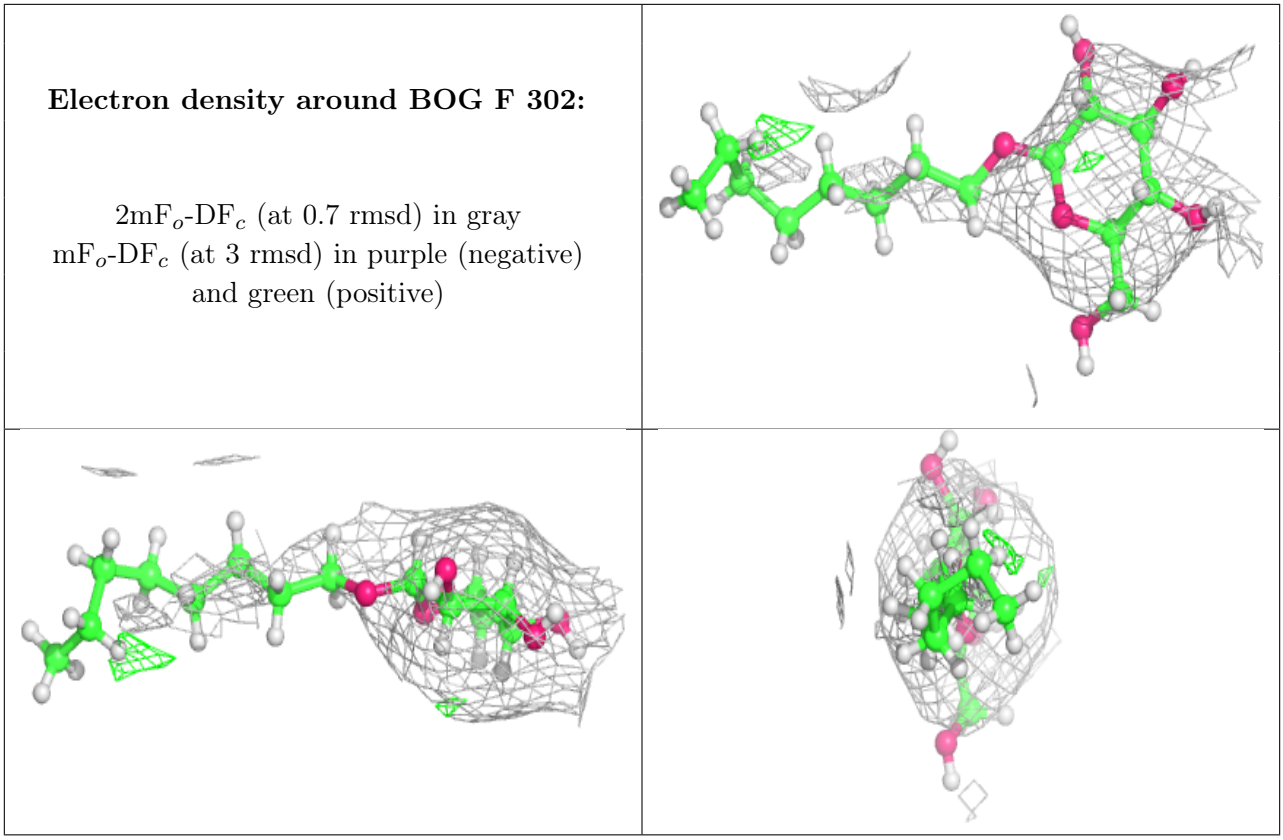






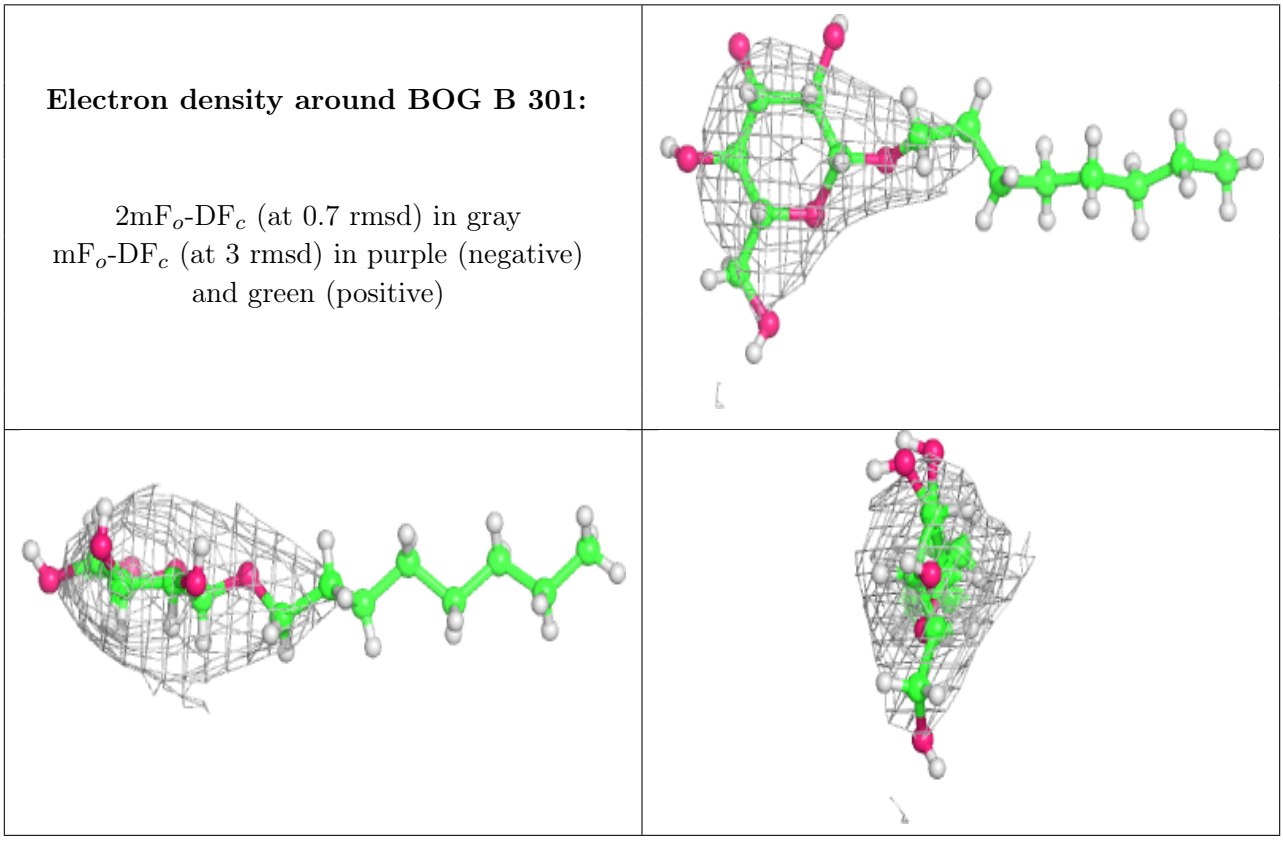
Electron density around BOG F 302:

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



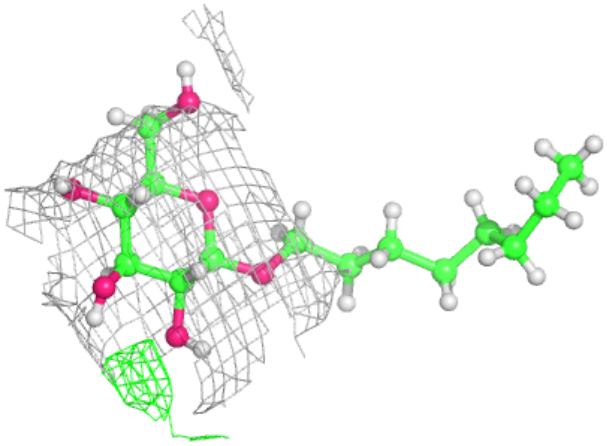
Electron density around BOG B 301:

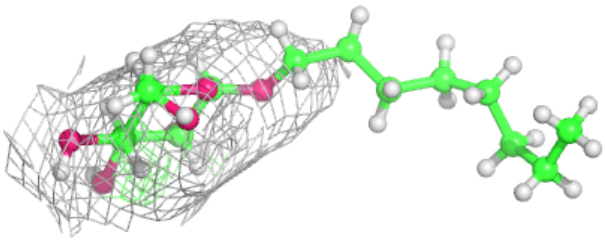
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

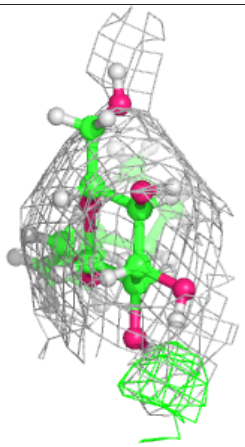


Electron density around BOG A 306:

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

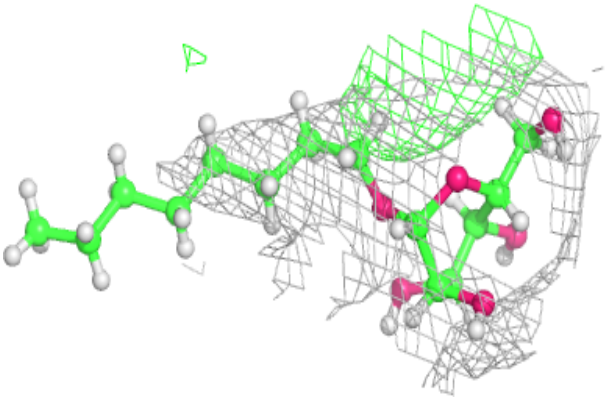


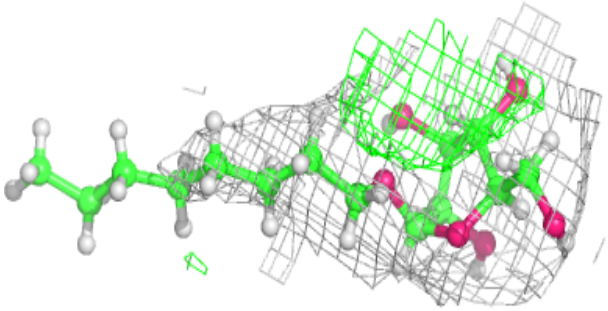


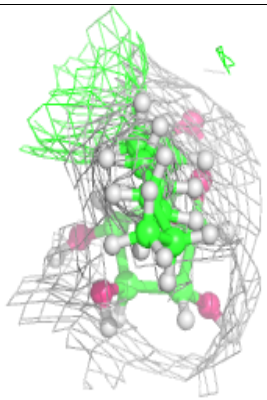


Electron density around BOG D 301:

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

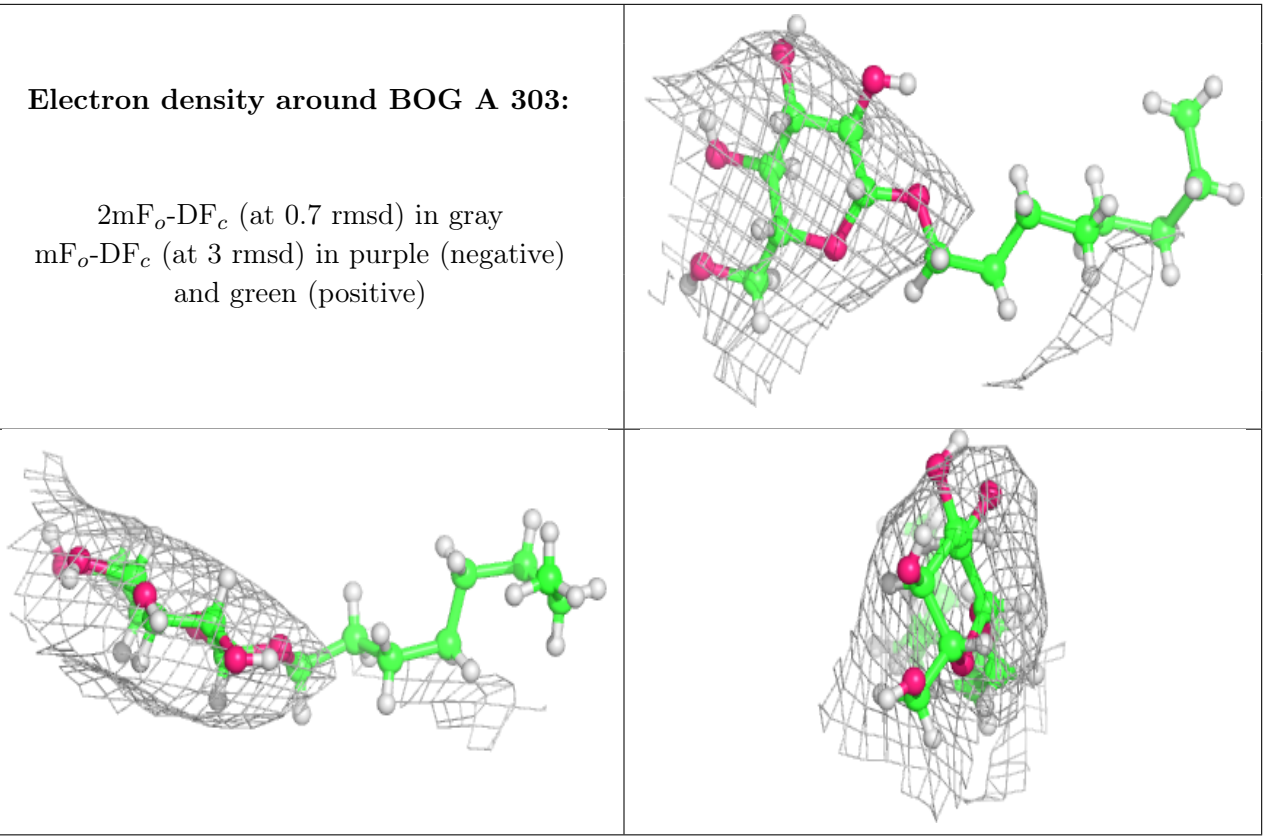






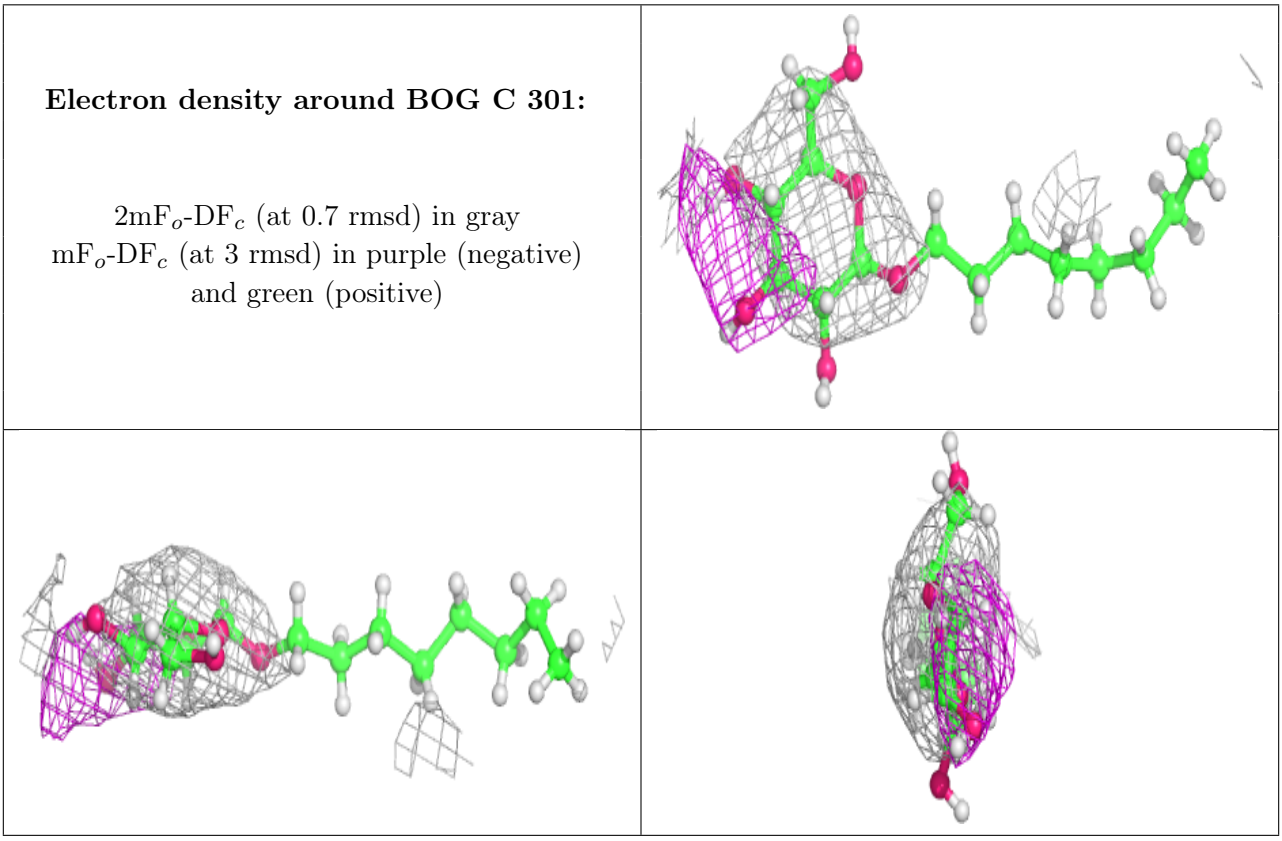
Electron density around BOG A 303:

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



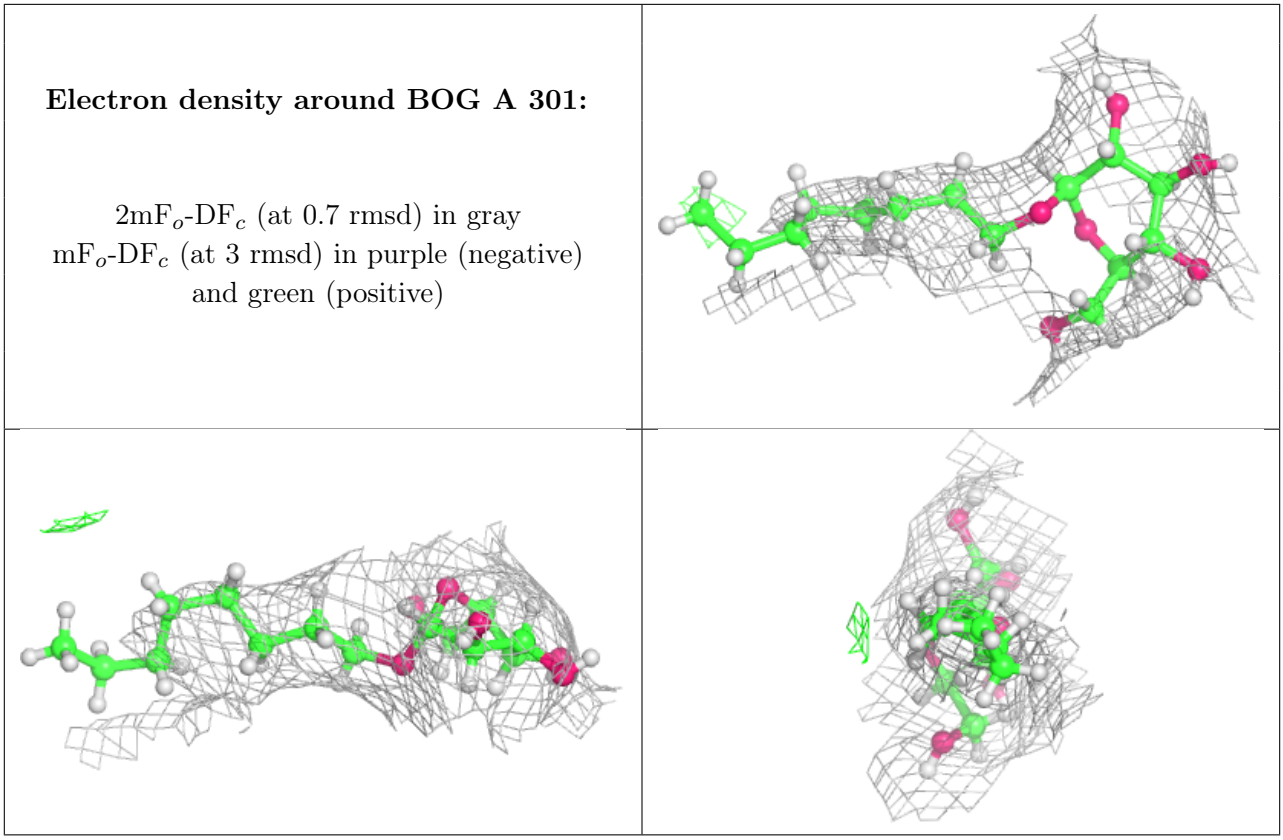
Electron density around BOG C 301:

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



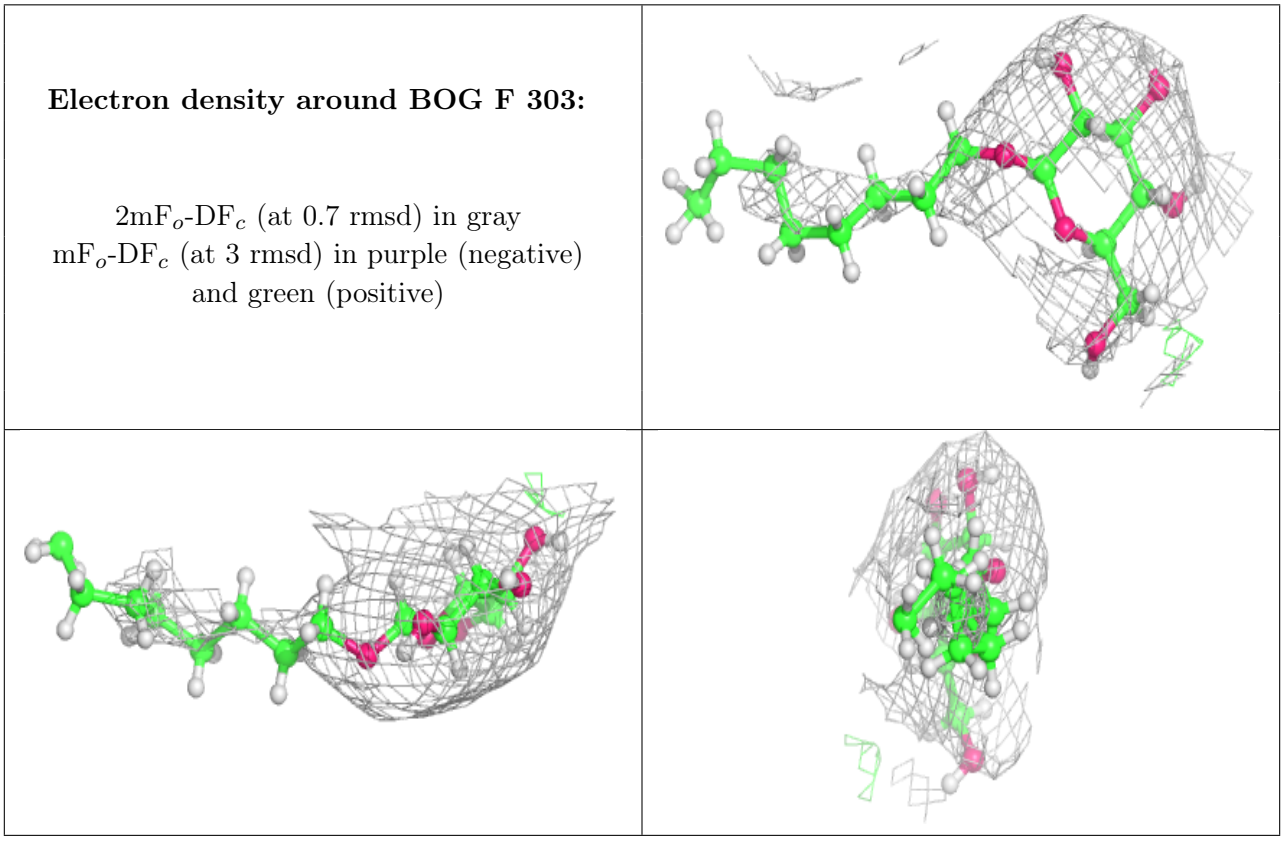
Electron density around BOG A 301:

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



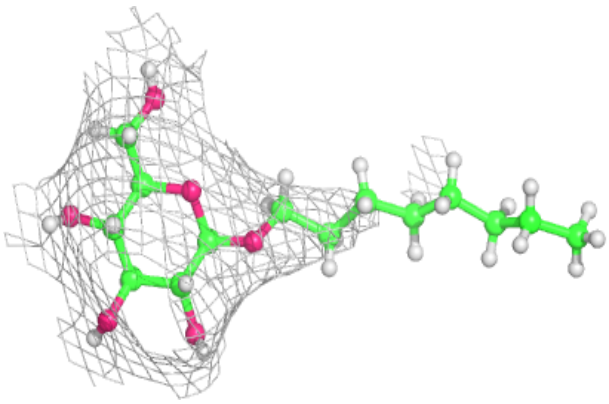
Electron density around BOG F 303:

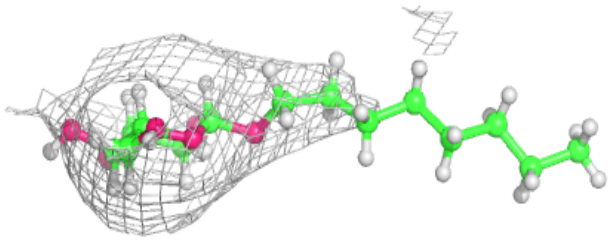
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

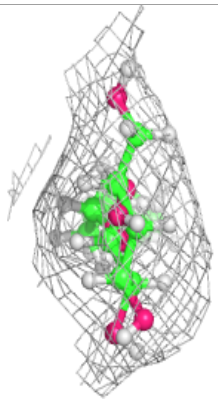


Electron density around BOG A 304:

$2mF_o$-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.