Full wwPDB X-ray Structure Validation Report (i)

Dec 15, 2024 – 12:08 PM JST

PDB ID	:	8XUA
Title	:	Oligogalacturonate-specific porin from Vibrio harveyi (VhGalP)
Authors	:	Meesrikaew, P.; Sanram, S.; Robinson, R.; Suginta, W.
Deposited on	:	2024-01-12
Resolution	:	2.70 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:

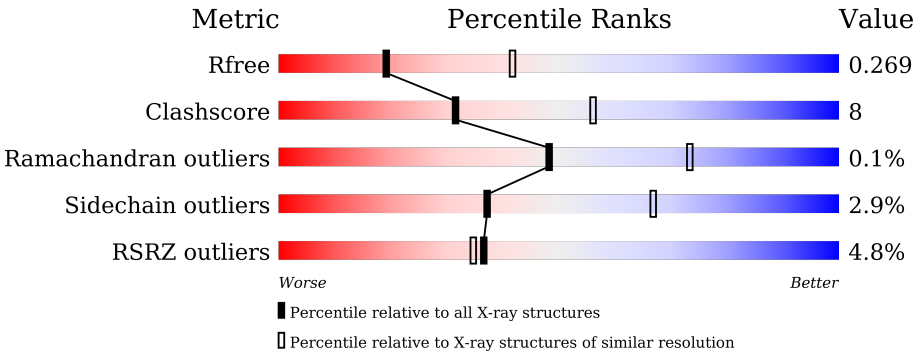
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	210	86% 13%
1	B	210	90% 9%
1	C	210	84% 15%
1	D	210	16% 74% 24%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	301	-	-	X	-

2 Entry composition

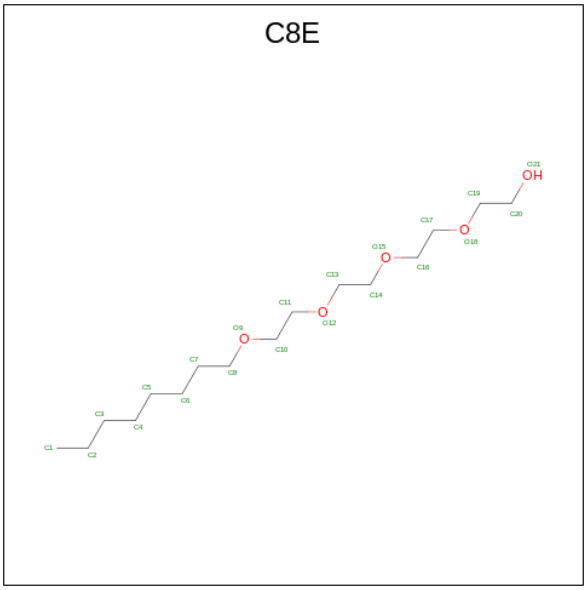
There are 5 unique types of molecules in this entry. The entry contains 6855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1634	1018	282	329	5			
1	B	210	Total	C	N	O	S	0	0	0
			1634	1018	282	329	5			
1	C	210	Total	C	N	O	S	0	0	0
			1634	1018	282	329	5			
1	D	210	Total	C	N	O	S	0	0	0
			1631	1015	282	329	5			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			15	10	5		

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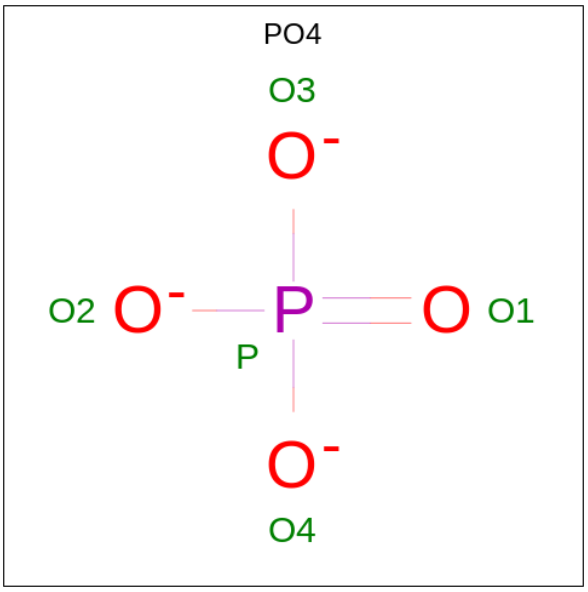
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 16 5	0	0
2	A	1	Total C O 12 8 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	B	1	Total C O 21 16 5	0	0
2	B	1	Total C O 12 8 4	0	0
2	B	1	Total C O 11 7 4	0	0
2	B	1	Total C O 11 7 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	B	1	Total C O 21 16 5	0	0
2	B	1	Total C O 11 7 4	0	0
2	B	1	Total C O 9 6 3	0	0
2	C	1	Total C O 16 11 5	0	0
2	C	1	Total C O 6 4 2	0	0
2	C	1	Total C O 12 8 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	C	1	Total C O 12 8 4	0	0
2	D	1	Total C O 6 4 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

- Molecule 5 is water.

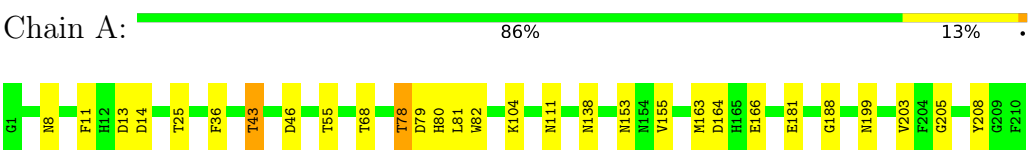
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	29	Total O 29 29	0	0
5	C	10	Total O 10 10	0	0
5	D	5	Total O 5 5	0	0

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.

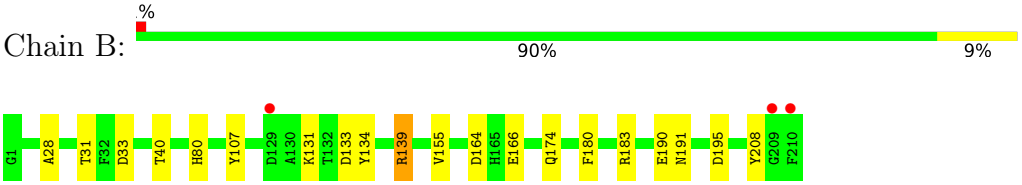
• Molecule 1: Porin

Chain A:



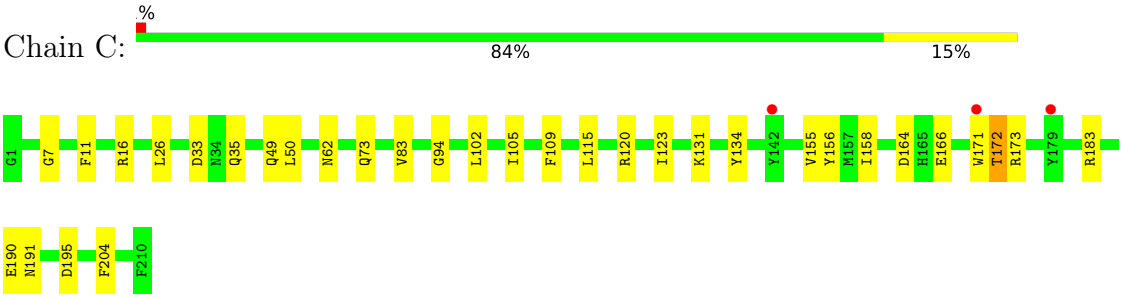
• Molecule 1: Porin

Chain B:



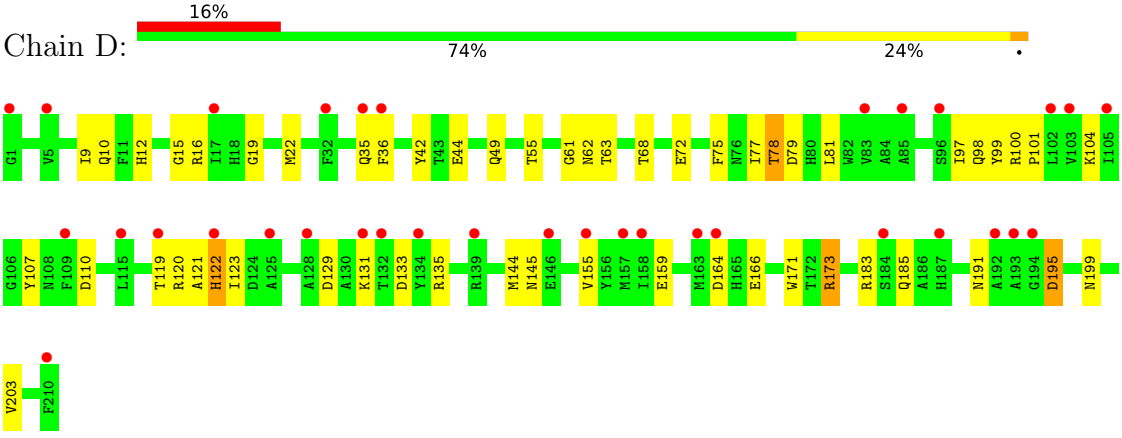
• Molecule 1: Porin

Chain C:



• Molecule 1: Porin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.54Å 77.09Å 143.06Å 90.00° 95.09° 90.00°	Depositor
Resolution (Å)	38.21 – 2.70 38.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.21-2.70) 98.8 (38.21-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.209 , 0.268 0.211 , 0.269	Depositor DCC
R_{free} test set	1656 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6855	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: C8E, NA, PO4

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	0.46	0/1673	0.67	0/2268
1	B	0.49	0/1673	0.68	0/2268
1	C	0.38	0/1673	0.60	0/2268
1	D	0.32	0/1670	0.56	0/2264
All	All	0.42	0/6689	0.63	0/9068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1634	0	1487	30	0
1	B	1634	0	1487	13	0
1	C	1634	0	1487	25	0
1	D	1631	0	1478	31	0
2	A	84	0	120	22	0
2	B	106	0	146	4	0
2	C	56	0	70	5	0
2	D	6	0	6	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	19	0	0	1	0
5	B	29	0	0	1	0
5	C	10	0	0	0	0
5	D	5	0	0	0	0
All	All	6855	0	6281	104	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 8.

All (104) 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:78:THR:HG22	1:A:81:LEU:H	1.38	0.88
2:A:301:C8E:H171	2:A:301:C8E:H11	1.57	0.84
1:B:155:VAL:HB	1:B:164:ASP:HB2	1.64	0.79
1:D:78:THR:HG23	1:D:81:LEU:HB3	1.65	0.78
1:A:155:VAL:HB	1:A:164:ASP:HB2	1.68	0.76
1:C:155:VAL:HB	1:C:164:ASP:HB2	1.67	0.76
1:C:191:ASN:HD21	1:C:195:ASP:HB2	1.51	0.75
1:A:188:GLY:HA2	1:C:35:GLN:HE22	1.50	0.75
1:A:13:ASP:HB3	2:A:305:C8E:H102	1.72	0.70
1:A:104:LYS:HE2	2:A:301:C8E:H131	1.75	0.69
1:A:138:ASN:HB3	2:A:303:C8E:H192	1.75	0.69
1:D:10:GLN:HG2	1:D:203:VAL:HG22	1.76	0.68
1:C:83:VAL:HG12	1:C:105:ILE:HG13	1.80	0.63
1:D:166:GLU:HG2	1:D:183:ARG:HG2	1.79	0.62
1:A:111:ASN:ND2	1:C:134:TYR:OH	2.34	0.61
2:A:301:C8E:H171	2:A:301:C8E:C1	2.30	0.61
1:C:166:GLU:HG2	1:C:183:ARG:HG2	1.84	0.59
1:D:171:TRP:HE1	1:D:173:ARG:HB3	1.67	0.59
1:D:171:TRP:NE1	1:D:173:ARG:HB3	2.19	0.58
1:A:104:LYS:HD3	2:A:301:C8E:H102	1.86	0.57
1:A:78:THR:HG23	1:A:80:HIS:H	1.69	0.56
1:A:104:LYS:NZ	2:A:301:C8E:H71	2.21	0.56
1:A:153:ASN:HB3	1:A:166:GLU:HB2	1.86	0.56
1:C:62:ASN:O	1:D:62:ASN:ND2	2.39	0.55
1:C:109:PHE:HE1	1:C:115:LEU:CD1	2.19	0.55
1:C:171:TRP:NE1	1:C:173:ARG:HB3	2.22	0.55
1:D:155:VAL:HB	1:D:164:ASP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLN:HG2	1:D:36:PHE:CD2	2.42	0.54
1:B:166:GLU:HG2	1:B:183:ARG:HG2	1.90	0.53
1:C:191:ASN:ND2	1:C:195:ASP:HB2	2.22	0.52
2:A:301:C8E:H11	2:A:301:C8E:H192	1.90	0.52
1:A:188:GLY:HA2	1:C:35:GLN:NE2	2.21	0.52
2:A:303:C8E:H22	1:C:73:GLN:NE2	2.25	0.52
1:B:180:PHE:HB2	2:B:304:C8E:H201	1.91	0.51
1:D:81:LEU:HB2	1:D:107:TYR:HD2	1.75	0.51
1:A:78:THR:CG2	1:A:80:HIS:H	2.23	0.51
1:B:139:ARG:NH1	5:B:403:HOH:O	2.44	0.51
1:A:138:ASN:HB3	2:A:303:C8E:H161	1.92	0.51
1:C:172:THR:O	1:C:172:THR:OG1	2.23	0.50
1:D:15:GLY:O	1:D:19:GLY:N	2.45	0.49
1:D:72:GLU:OE1	1:D:104:LYS:NZ	2.27	0.49
2:A:301:C8E:H72	5:A:409:HOH:O	2.13	0.49
1:A:78:THR:HG22	1:A:81:LEU:N	2.19	0.49
1:C:94:GLY:HA2	2:C:305:C8E:H112	1.94	0.49
1:C:109:PHE:HE1	1:C:115:LEU:HD11	1.77	0.48
1:D:100:ARG:HA	1:D:121:ALA:O	2.13	0.48
1:A:104:LYS:HZ2	2:A:301:C8E:H71	1.78	0.47
1:C:94:GLY:HA2	2:C:305:C8E:H132	1.96	0.47
1:D:120:ARG:HE	1:D:122:HIS:HE1	1.62	0.47
1:D:77:ILE:HG22	1:D:78:THR:HG22	1.96	0.47
1:A:78:THR:HG23	1:A:79:ASP:N	2.30	0.47
1:A:181:GLU:HB3	1:A:203:VAL:HB	1.97	0.47
1:C:49:GLN:O	1:C:50:LEU:HD23	2.14	0.47
1:D:10:GLN:HB3	1:D:12:HIS:CE1	2.50	0.46
1:A:82:TRP:HH2	2:A:301:C8E:H111	1.79	0.46
2:A:302:C8E:H82	2:C:301:C8E:H132	1.97	0.46
1:D:36:PHE:HD1	1:D:75:PHE:CE2	2.34	0.46
2:A:301:C8E:H71	2:A:301:C8E:H31	1.97	0.46
1:D:49:GLN:NE2	1:D:63:THR:H	2.14	0.46
1:A:82:TRP:CH2	2:A:301:C8E:H111	2.52	0.45
1:C:156:TYR:CE2	1:C:158:ILE:HA	2.52	0.45
1:A:208:TYR:HE2	1:B:208:TYR:HE2	1.64	0.45
1:C:123:ILE:HG21	2:C:304:C8E:H131	1.99	0.45
1:A:11:PHE:HB3	2:A:305:C8E:H131	1.99	0.44
1:D:99:TYR:HB2	1:D:123:ILE:HB	1.98	0.44
1:C:102:LEU:HB3	1:C:120:ARG:HG3	2.00	0.44
1:D:101:PRO:HD2	1:D:121:ALA:HB3	1.98	0.44
1:D:97:ILE:HG22	1:D:98:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:THR:HA	1:D:135:ARG:O	2.17	0.44
2:B:306:C8E:H141	2:B:306:C8E:H171	1.66	0.44
1:A:25:THR:HG23	1:A:46:ASP:HA	2.00	0.43
1:B:80:HIS:O	1:B:107:TYR:HA	2.17	0.43
2:B:304:C8E:H161	2:B:305:C8E:H162	2.00	0.43
1:D:49:GLN:HE22	1:D:63:THR:H	1.66	0.43
1:A:14:ASP:O	1:A:199:ASN:OD1	2.37	0.43
1:A:43:THR:HA	1:A:68:THR:O	2.18	0.43
1:D:22:MET:HE2	1:D:22:MET:HB2	1.86	0.43
1:D:185:GLN:OE1	1:D:199:ASN:ND2	2.46	0.43
1:C:190:GLU:HA	1:C:195:ASP:O	2.19	0.42
1:D:144:MET:HG2	1:D:145:ASN:ND2	2.34	0.42
2:A:302:C8E:H82	2:C:301:C8E:H111	2.01	0.42
1:A:8:ASN:HA	1:A:205:GLY:HA2	2.00	0.42
1:A:104:LYS:CD	2:A:301:C8E:H102	2.49	0.42
1:C:16:ARG:HG3	1:C:16:ARG:HH11	1.84	0.42
1:A:104:LYS:HZ2	2:A:301:C8E:H102	1.84	0.42
1:D:191:ASN:OD1	1:D:195:ASP:N	2.51	0.42
1:C:7:GLY:HA3	1:C:26:LEU:HD23	2.02	0.41
1:B:133:ASP:OD1	1:B:134:TYR:N	2.47	0.41
1:C:11:PHE:CD2	1:C:204:PHE:HE2	2.37	0.41
2:A:301:C8E:H11	2:A:301:C8E:C17	2.41	0.41
1:B:191:ASN:HD21	1:B:195:ASP:HB2	1.85	0.41
1:D:55:THR:HG22	1:D:61:GLY:HA2	2.03	0.41
1:B:190:GLU:HA	1:B:195:ASP:O	2.20	0.41
1:D:44:GLU:HB3	1:D:68:THR:HB	2.02	0.41
1:A:104:LYS:NZ	2:A:301:C8E:C10	2.84	0.41
1:B:191:ASN:ND2	1:B:195:ASP:HB2	2.36	0.41
1:B:28:ALA:HB2	2:B:301:C8E:H61	2.03	0.41
1:B:31:THR:HA	1:B:40:THR:HA	2.02	0.41
1:B:174:GLN:H	1:B:174:GLN:HG2	1.70	0.41
1:C:16:ARG:HG3	1:C:16:ARG:NH1	2.36	0.41
1:D:36:PHE:CD1	1:D:75:PHE:HE2	2.39	0.41
1:D:133:ASP:OD2	1:D:159:GLU:HB2	2.21	0.41
1:D:9:ILE:HD13	1:D:9:ILE:HA	1.86	0.40
1:A:155:VAL:O	1:A:163:MET:HA	2.21	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	208/210 (99%)	205 (99%)	3 (1%)	0	100	100
1	B	208/210 (99%)	203 (98%)	5 (2%)	0	100	100
1	C	208/210 (99%)	205 (99%)	3 (1%)	0	100	100
1	D	208/210 (99%)	193 (93%)	14 (7%)	1 (0%)	25	49
All	All	832/840 (99%)	806 (97%)	25 (3%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	129	ASP

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	166/166 (100%)	162 (98%)	4 (2%)	44	73
1	B	166/166 (100%)	163 (98%)	3 (2%)	54	80
1	C	166/166 (100%)	163 (98%)	3 (2%)	54	80
1	D	165/166 (99%)	156 (94%)	9 (6%)	18	41
All	All	663/664 (100%)	644 (97%)	19 (3%)	37	67

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	43	THR
1	A	55	THR
1	A	78	THR
1	B	33	ASP
1	B	131	LYS
1	B	139	ARG
1	C	33	ASP
1	C	131	LYS
1	C	172	THR
1	D	16	ARG
1	D	42	TYR
1	D	78	THR
1	D	79	ASP
1	D	110	ASP
1	D	122	HIS
1	D	131	LYS
1	D	173	ARG
1	D	195	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	GLN
1	C	73	GLN
1	D	49	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	C8E	B	306	-	20,20,20	0.50	0	19,19,19	0.46	0
2	C8E	A	305	-	14,14,20	0.50	0	13,13,19	0.23	0
2	C8E	B	303	-	10,10,20	0.45	0	9,9,19	0.41	0
2	C8E	B	305	-	9,9,20	0.45	0	8,8,19	0.35	0
2	C8E	C	302	-	5,5,20	0.46	0	4,4,19	0.37	0
2	C8E	C	301	-	15,15,20	0.42	0	14,14,19	0.26	0
2	C8E	D	301	-	5,5,20	0.47	0	4,4,19	0.06	0
2	C8E	A	301	-	20,20,20	1.33	4 (20%)	19,19,19	0.64	0
2	C8E	B	302	-	11,11,20	0.47	0	10,10,19	0.36	0
2	C8E	C	303	-	11,11,20	0.54	0	10,10,19	0.28	0
2	C8E	C	304	-	9,9,20	0.44	0	8,8,19	0.28	0
3	PO4	B	309	-	4,4,4	1.03	0	6,6,6	0.47	0
2	C8E	A	302	-	14,14,20	0.49	0	13,13,19	0.31	0
2	C8E	B	307	-	10,10,20	0.49	0	9,9,19	0.61	0
2	C8E	B	304	-	10,10,20	0.44	0	9,9,19	0.56	0
2	C8E	B	308	-	8,8,20	0.49	0	7,7,19	0.18	0
2	C8E	B	301	-	20,20,20	0.60	0	19,19,19	0.57	0
2	C8E	C	305	-	11,11,20	0.48	0	10,10,19	0.29	0
2	C8E	A	303	-	20,20,20	0.37	0	19,19,19	0.47	0
2	C8E	A	304	-	11,11,20	0.48	0	10,10,19	0.25	0

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	C8E	B	306	-	-	12/18/18/18	-
2	C8E	A	305	-	-	9/12/12/18	-
2	C8E	B	303	-	-	3/8/8/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	B	305	-	-	3/7/7/18	-
2	C8E	C	302	-	-	2/3/3/18	-
2	C8E	C	301	-	-	9/13/13/18	-
2	C8E	D	301	-	-	2/3/3/18	-
2	C8E	A	301	-	-	11/18/18/18	-
2	C8E	B	302	-	-	6/9/9/18	-
2	C8E	C	303	-	-	7/9/9/18	-
2	C8E	C	304	-	-	4/7/7/18	-
2	C8E	A	302	-	-	10/12/12/18	-
2	C8E	B	307	-	-	2/8/8/18	-
2	C8E	B	304	-	-	4/8/8/18	-
2	C8E	B	308	-	-	5/6/6/18	-
2	C8E	B	301	-	-	8/18/18/18	-
2	C8E	C	305	-	-	8/9/9/18	-
2	C8E	A	303	-	-	13/18/18/18	-
2	C8E	A	304	-	-	5/9/9/18	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	C8E	C14-C13	2.48	1.61	1.49
2	A	301	C8E	C19-C20	2.42	1.62	1.49
2	A	301	C8E	C17-C16	2.13	1.60	1.49
2	A	301	C8E	O18-C19	2.07	1.51	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	306	C8E	C17-C16-O15-C14
2	B	301	C8E	C3-C4-C5-C6
2	A	301	C8E	O12-C13-C14-O15
2	A	303	C8E	O9-C10-C11-O12
2	B	303	C8E	O12-C13-C14-O15
2	C	301	C8E	O9-C10-C11-O12
2	A	301	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
2	B	301	C8E	O15-C16-C17-O18
2	C	301	C8E	O15-C16-C17-O18
2	C	303	C8E	O12-C13-C14-O15
2	A	304	C8E	O12-C13-C14-O15
2	B	301	C8E	O12-C13-C14-O15
2	B	304	C8E	O15-C16-C17-O18
2	B	308	C8E	O15-C16-C17-O18
2	A	302	C8E	O12-C13-C14-O15
2	A	305	C8E	C6-C7-C8-O9
2	A	303	C8E	O15-C16-C17-O18
2	B	304	C8E	O18-C19-C20-O21
2	C	301	C8E	O18-C19-C20-O21
2	C	305	C8E	O18-C19-C20-O21
2	C	301	C8E	O12-C13-C14-O15
2	B	306	C8E	C6-C7-C8-O9
2	B	305	C8E	O15-C16-C17-O18
2	B	301	C8E	O18-C19-C20-O21
2	B	305	C8E	O18-C19-C20-O21
2	B	308	C8E	O18-C19-C20-O21
2	A	305	C8E	C14-C13-O12-C11
2	B	301	C8E	C4-C5-C6-C7
2	A	301	C8E	C4-C5-C6-C7
2	A	301	C8E	C17-C16-O15-C14
2	B	306	C8E	C2-C3-C4-C5
2	B	302	C8E	O12-C13-C14-O15
2	A	302	C8E	O18-C19-C20-O21
2	A	301	C8E	C2-C3-C4-C5
2	A	305	C8E	O12-C13-C14-O15
2	A	304	C8E	O15-C16-C17-O18
2	C	305	C8E	O12-C13-C14-O15
2	C	304	C8E	O18-C19-C20-O21
2	C	303	C8E	O15-C16-C17-O18
2	A	303	C8E	C6-C7-C8-O9
2	A	303	C8E	O12-C13-C14-O15
2	C	302	C8E	O9-C10-C11-O12
2	B	302	C8E	O18-C19-C20-O21
2	B	303	C8E	O18-C19-C20-O21
2	C	304	C8E	O12-C13-C14-O15
2	C	305	C8E	C17-C16-O15-C14
2	B	307	C8E	O12-C13-C14-O15
2	A	302	C8E	C7-C8-O9-C10
2	A	305	C8E	O15-C16-C17-O18

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Mol	Chain	Res	Type	Atoms
2	C	305	C8E	O15-C16-C17-O18
2	A	303	C8E	C3-C4-C5-C6
2	A	305	C8E	O9-C10-C11-O12
2	C	305	C8E	C10-C11-O12-C13
2	B	303	C8E	C14-C13-O12-C11
2	D	301	C8E	O9-C10-C11-O12
2	B	306	C8E	O15-C16-C17-O18
2	C	302	C8E	C14-C13-O12-C11
2	B	308	C8E	C20-C19-O18-C17
2	A	302	C8E	C20-C19-O18-C17
2	B	306	C8E	C13-C14-O15-C16
2	C	301	C8E	C13-C14-O15-C16
2	C	305	C8E	C20-C19-O18-C17
2	B	304	C8E	C17-C16-O15-C14
2	A	305	C8E	C13-C14-O15-C16
2	B	302	C8E	C13-C14-O15-C16
2	C	305	C8E	C16-C17-O18-C19
2	A	304	C8E	C13-C14-O15-C16
2	A	305	C8E	C10-C11-O12-C13
2	C	301	C8E	C7-C8-O9-C10
2	A	305	C8E	C17-C16-O15-C14
2	C	301	C8E	C16-C17-O18-C19
2	A	301	C8E	C14-C13-O12-C11
2	A	303	C8E	C13-C14-O15-C16
2	B	306	C8E	C20-C19-O18-C17
2	A	303	C8E	O18-C19-C20-O21
2	B	306	C8E	O18-C19-C20-O21
2	A	303	C8E	C1-C2-C3-C4
2	A	302	C8E	C14-C13-O12-C11
2	C	304	C8E	C17-C16-O15-C14
2	B	306	C8E	C7-C8-O9-C10
2	A	301	C8E	C11-C10-O9-C8
2	A	305	C8E	C20-C19-O18-C17
2	B	308	C8E	C17-C16-O15-C14
2	C	303	C8E	C13-C14-O15-C16
2	D	301	C8E	C14-C13-O12-C11
2	A	301	C8E	O15-C16-C17-O18
2	A	302	C8E	C16-C17-O18-C19
2	A	301	C8E	C20-C19-O18-C17
2	C	301	C8E	C6-C7-C8-O9
2	A	302	C8E	C11-C10-O9-C8
2	B	308	C8E	C16-C17-O18-C19

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Mol	Chain	Res	Type	Atoms
2	C	303	C8E	C20-C19-O18-C17
2	B	301	C8E	C10-C11-O12-C13
2	A	303	C8E	C2-C3-C4-C5
2	B	302	C8E	C10-C11-O12-C13
2	C	305	C8E	C13-C14-O15-C16
2	B	306	C8E	C4-C5-C6-C7
2	A	301	C8E	C10-C11-O12-C13
2	A	304	C8E	C20-C19-O18-C17
2	B	305	C8E	C20-C19-O18-C17
2	B	306	C8E	C16-C17-O18-C19
2	A	302	C8E	C10-C11-O12-C13
2	A	303	C8E	C20-C19-O18-C17
2	B	304	C8E	O12-C13-C14-O15
2	C	301	C8E	C14-C13-O12-C11
2	A	301	C8E	C7-C8-O9-C10
2	A	302	C8E	O9-C10-C11-O12
2	B	306	C8E	C11-C10-O9-C8
2	A	303	C8E	C4-C5-C6-C7
2	C	303	C8E	C17-C16-O15-C14
2	A	303	C8E	C14-C13-O12-C11
2	C	303	C8E	C16-C17-O18-C19
2	C	304	C8E	C20-C19-O18-C17
2	B	301	C8E	O9-C10-C11-O12
2	B	306	C8E	C1-C2-C3-C4
2	C	303	C8E	C14-C13-O12-C11
2	A	302	C8E	O15-C16-C17-O18
2	A	303	C8E	C7-C8-O9-C10
2	B	307	C8E	O15-C16-C17-O18
2	B	302	C8E	O15-C16-C17-O18
2	B	301	C8E	C13-C14-O15-C16
2	A	304	C8E	C14-C13-O12-C11
2	B	302	C8E	C17-C16-O15-C14

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	306	C8E	1	0
2	A	305	C8E	2	0
2	B	305	C8E	1	0
2	C	301	C8E	2	0
2	A	301	C8E	15	0

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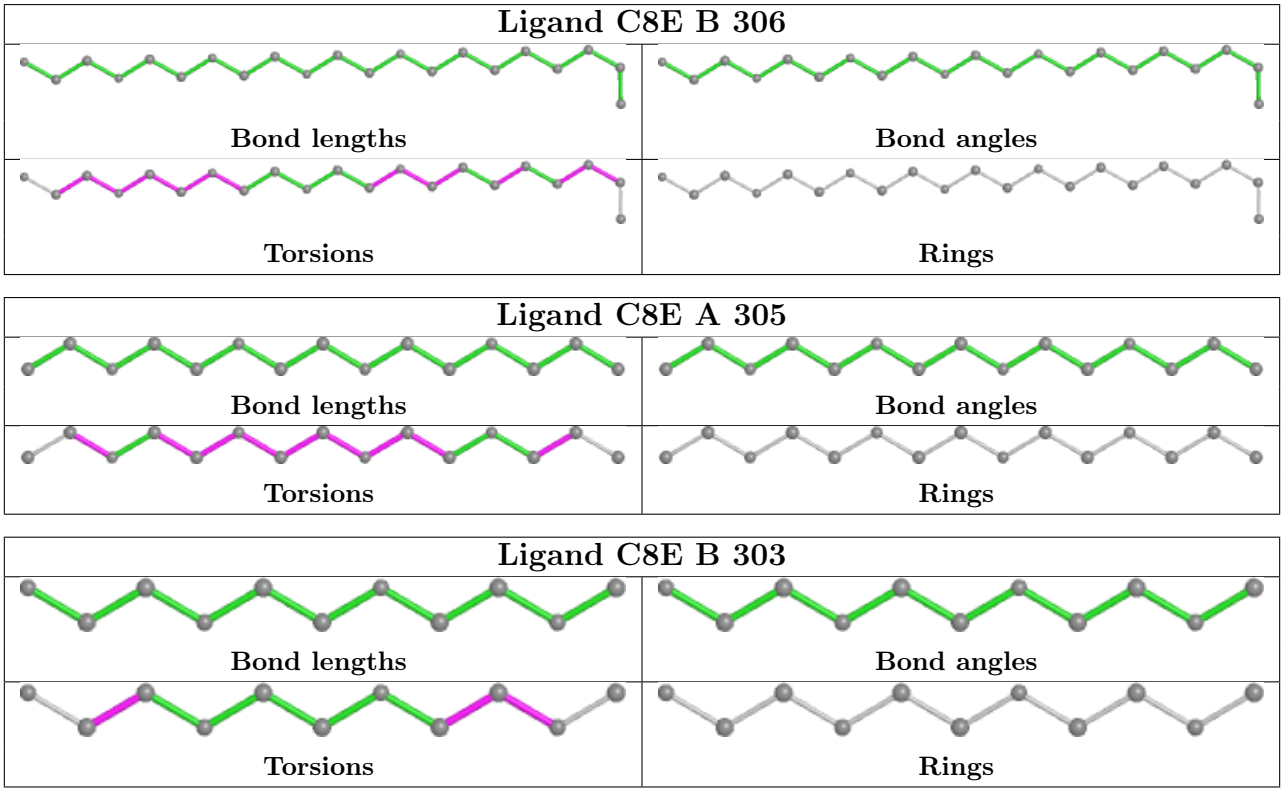
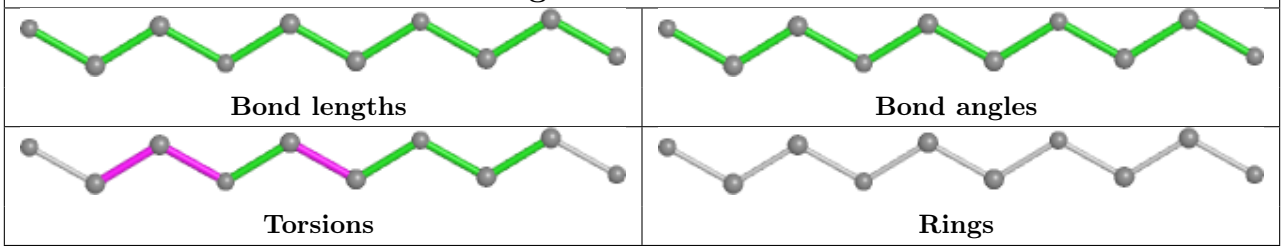
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	304	C8E	1	0
2	A	302	C8E	2	0
2	B	304	C8E	2	0
2	B	301	C8E	1	0
2	C	305	C8E	2	0
2	A	303	C8E	3	0

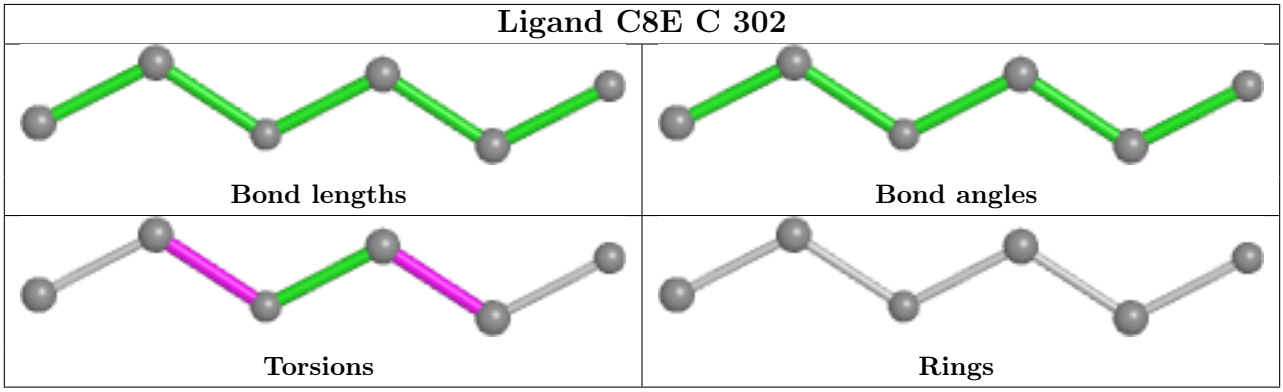
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



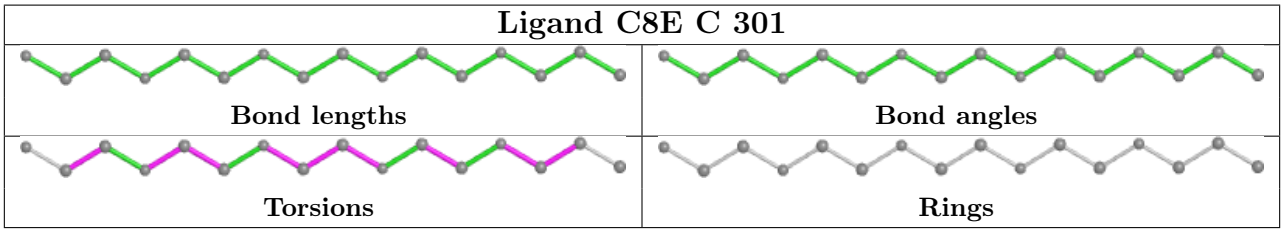
Ligand C8E B 305



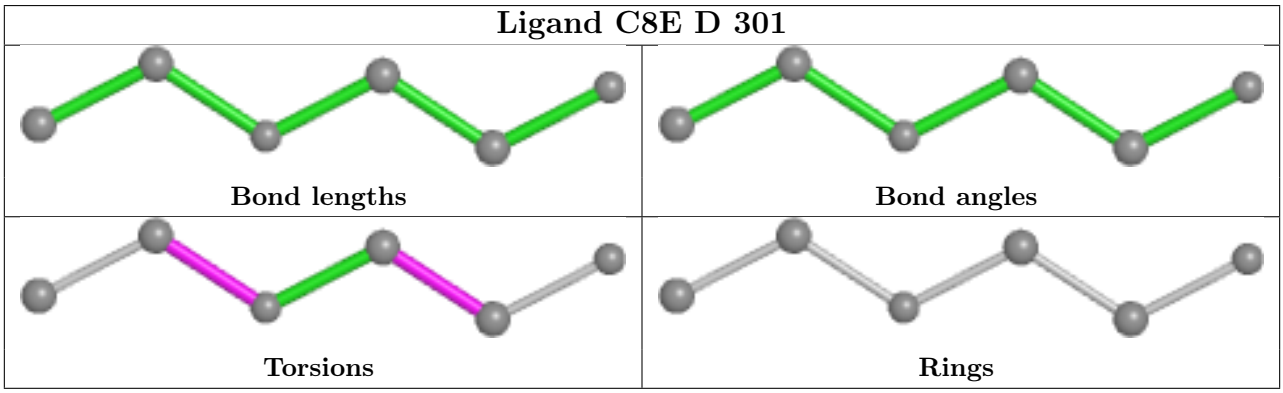
Ligand C8E C 302



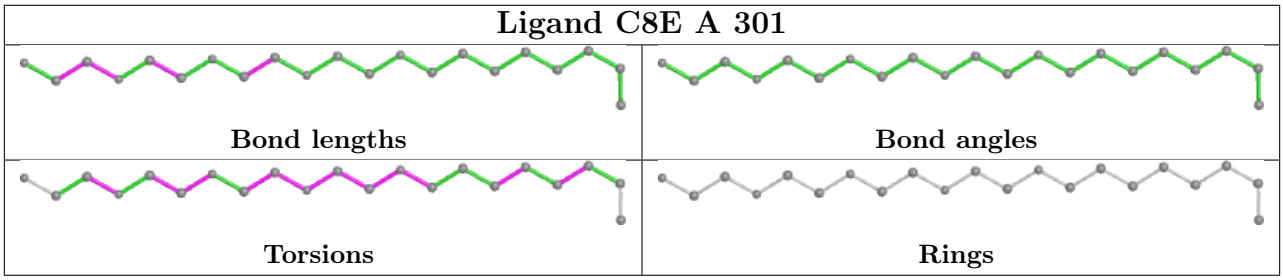
Ligand C8E C 301



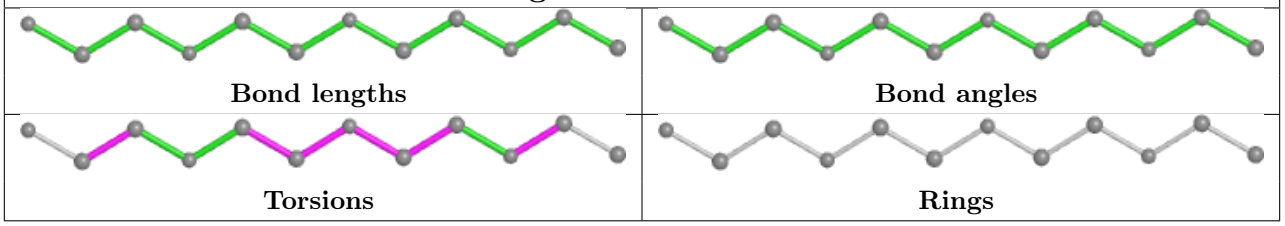
Ligand C8E D 301



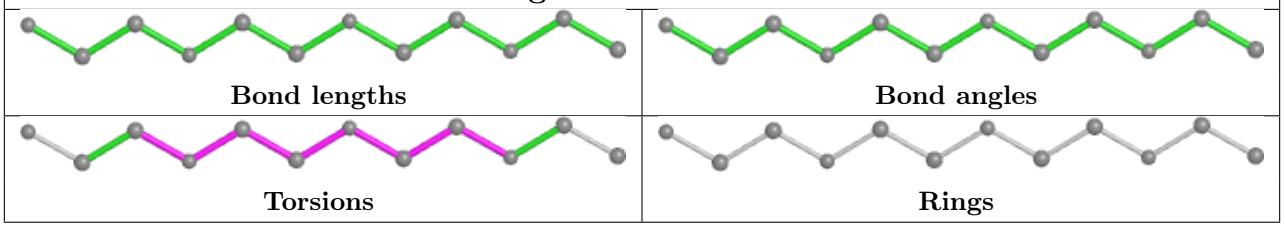
Ligand C8E A 301



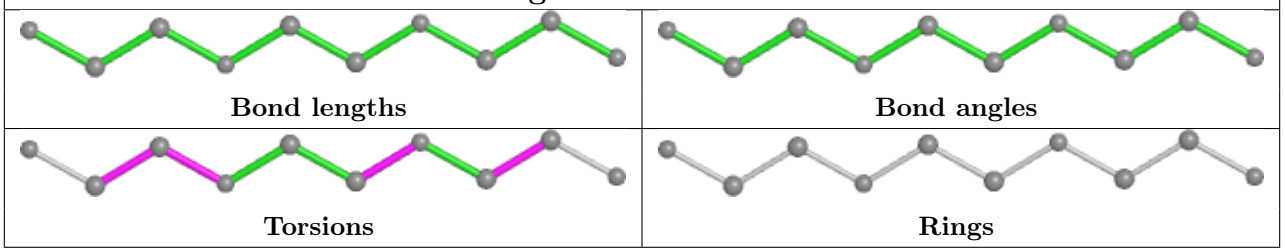
Ligand C8E B 302



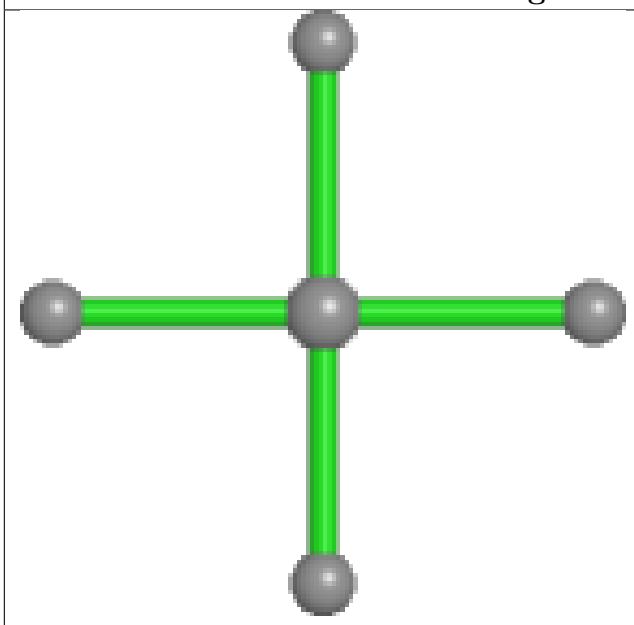
Ligand C8E C 303



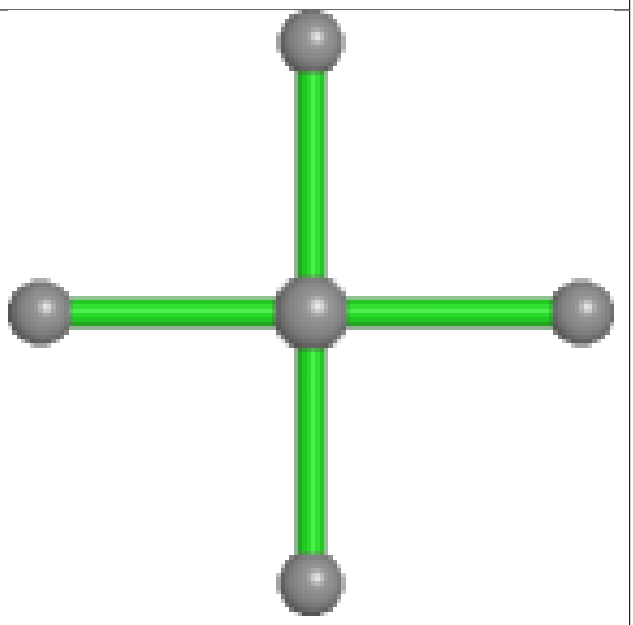
Ligand C8E C 304



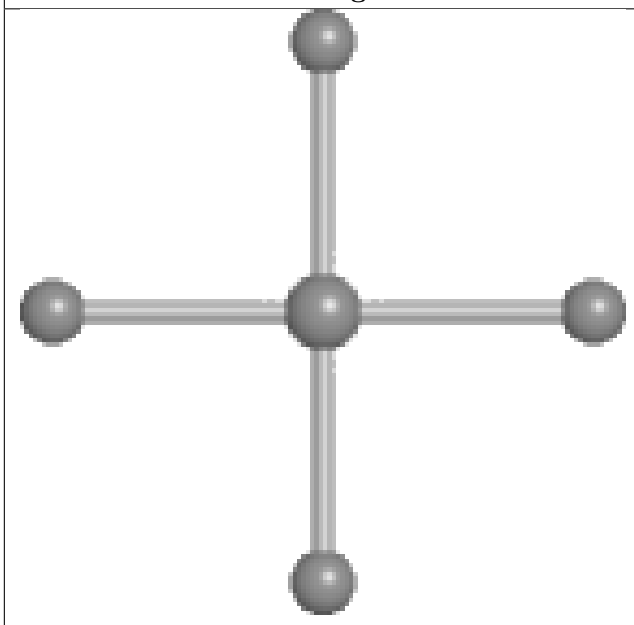
Ligand PO4 B 309



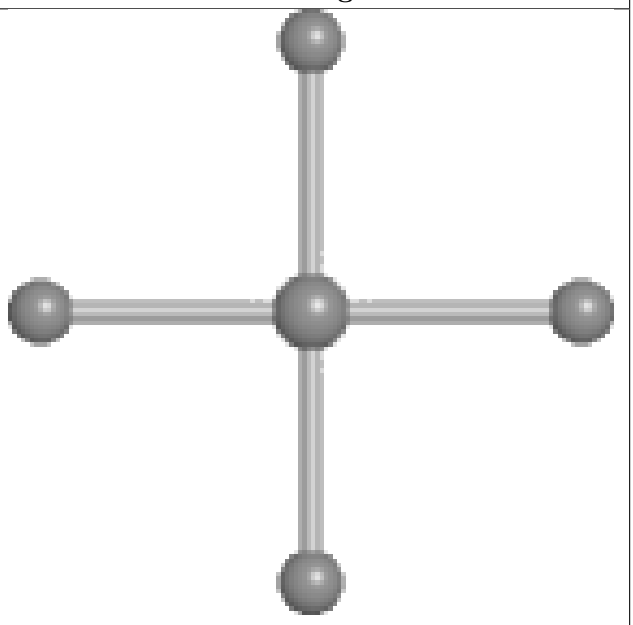
Bond lengths



Bond angles



Torsions



Rings

Ligand C8E A 302

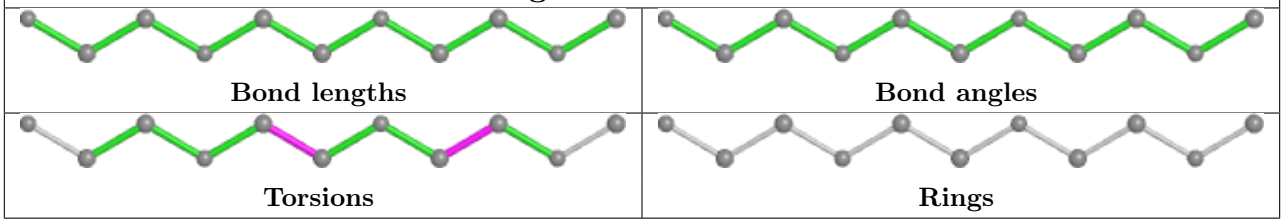
Bond lengths

Bond angles

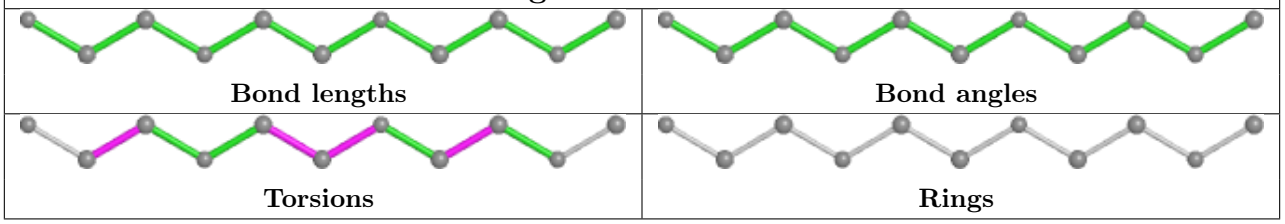
Torsions

Rings

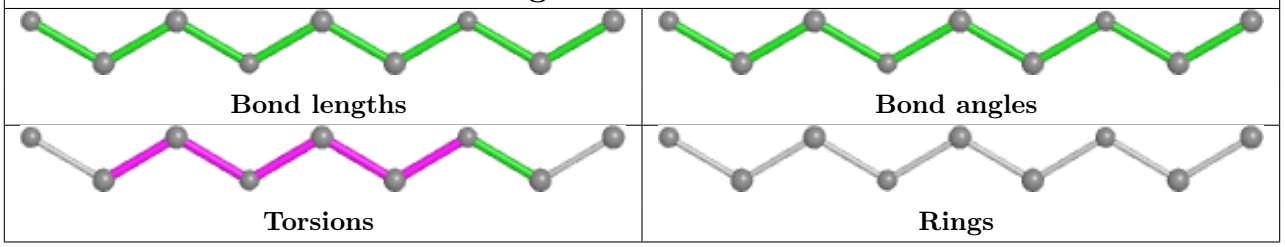
Ligand C8E B 307



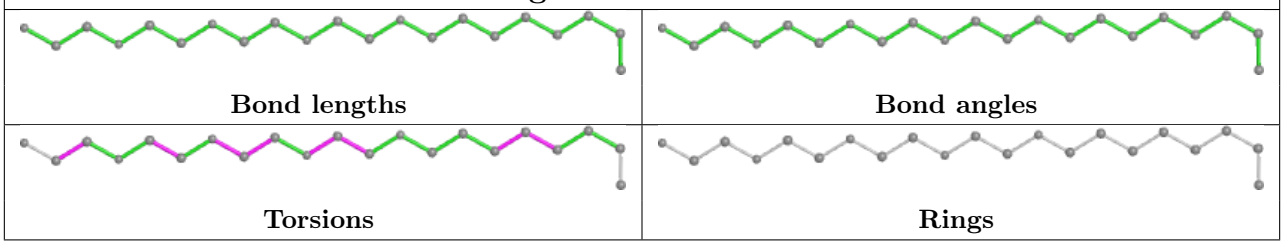
Ligand C8E B 304



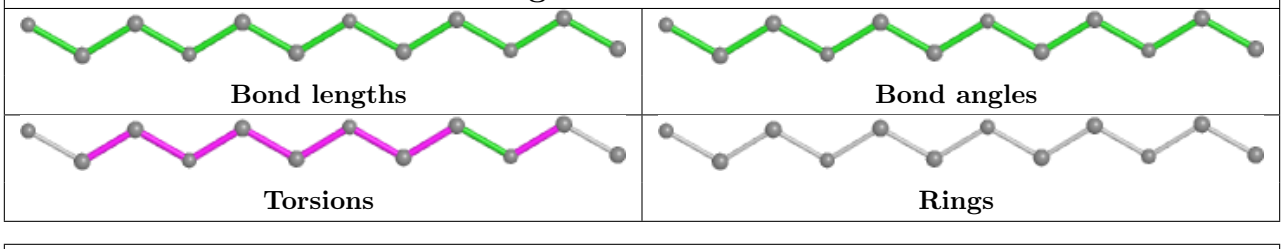
Ligand C8E B 308



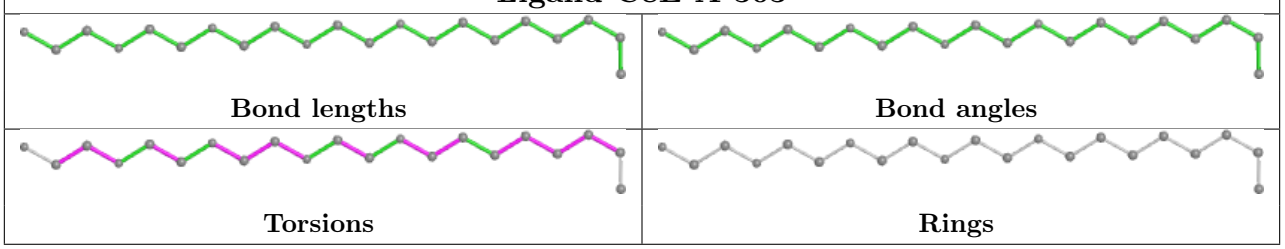
Ligand C8E B 301

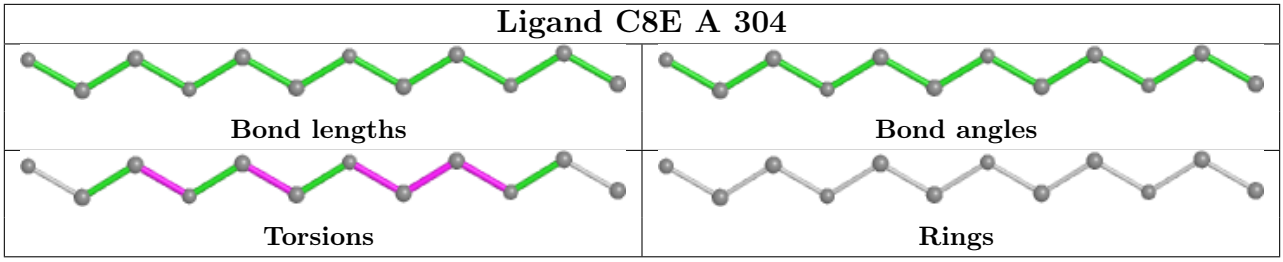


Ligand C8E C 305



Ligand C8E A 303





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	210/210 (100%)	-0.47	0 100 100	27, 40, 62, 95	0
1	B	210/210 (100%)	-0.47	3 (1%) 73 73	25, 36, 60, 75	0
1	C	210/210 (100%)	0.30	3 (1%) 73 73	42, 67, 92, 114	0
1	D	210/210 (100%)	1.17	34 (16%) 5 5	61, 96, 123, 142	0
All	All	840/840 (100%)	0.13	40 (4%) 36 35	25, 54, 111, 142	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	3.7
1	D	96	SER	3.3
1	D	17	ILE	3.2
1	D	134	TYR	3.2
1	D	32	PHE	3.1
1	D	163	MET	3.1
1	D	157	MET	3.0
1	D	210	PHE	3.0
1	D	187	HIS	2.9
1	D	83	VAL	2.8
1	D	146	GLU	2.8
1	B	210	PHE	2.8
1	D	184	SER	2.7
1	D	158	ILE	2.7
1	C	171	TRP	2.6
1	D	193	ALA	2.6
1	D	128	ALA	2.5
1	D	35	GLN	2.5
1	D	102	LEU	2.4
1	B	209	GLY	2.4
1	D	192	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	179	TYR	2.4
1	D	85	ALA	2.3
1	D	36	PHE	2.2
1	D	131	LYS	2.2
1	D	109	PHE	2.2
1	D	132	THR	2.2
1	D	103	VAL	2.2
1	D	115	LEU	2.2
1	D	194	GLY	2.2
1	D	119	THR	2.1
1	D	139	ARG	2.1
1	D	122	HIS	2.1
1	D	105	ILE	2.1
1	D	5	VAL	2.0
1	D	155	VAL	2.0
1	B	129	ASP	2.0
1	C	142	TYR	2.0
1	D	164	ASP	2.0
1	D	125	ALA	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	C8E	C	305	12/21	0.84	0.17	65,72,77,79	0
2	C8E	C	303	12/21	0.85	0.17	55,64,69,69	0
2	C8E	A	303	21/21	0.85	0.16	38,49,58,63	0
2	C8E	A	301	21/21	0.86	0.16	42,48,59,61	0

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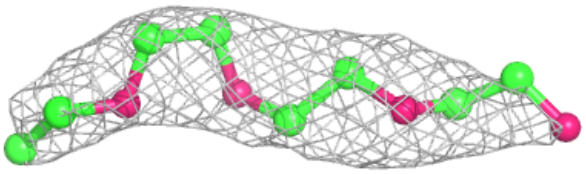
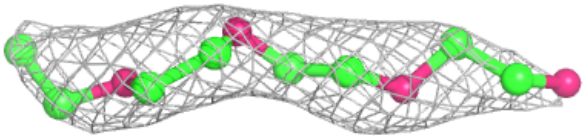
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	C8E	B	306	21/21	0.86	0.16	42,50,59,64	0
4	NA	C	306	1/1	0.86	0.26	57,57,57,57	0
2	C8E	A	305	15/21	0.87	0.14	42,56,61,64	0
2	C8E	A	304	12/21	0.87	0.12	49,59,67,68	0
2	C8E	B	307	11/21	0.87	0.17	40,47,53,53	0
2	C8E	D	301	6/21	0.88	0.19	66,71,73,74	0
2	C8E	C	304	10/21	0.88	0.13	65,75,79,80	0
2	C8E	C	301	16/21	0.89	0.14	43,53,63,64	0
2	C8E	B	301	21/21	0.90	0.13	32,40,51,52	0
2	C8E	B	302	12/21	0.90	0.11	44,52,58,61	0
2	C8E	B	308	9/21	0.91	0.12	44,48,57,61	0
2	C8E	B	305	10/21	0.92	0.10	46,50,56,57	0
2	C8E	A	302	15/21	0.92	0.12	45,58,63,68	0
2	C8E	C	302	6/21	0.92	0.20	62,65,68,68	0
2	C8E	B	304	11/21	0.92	0.13	37,43,54,55	0
2	C8E	B	303	11/21	0.93	0.11	40,50,55,65	0
3	PO4	B	309	5/5	0.96	0.07	42,44,47,53	0
4	NA	B	310	1/1	0.99	0.07	21,21,21,21	0

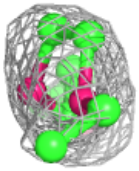
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E C 305:

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

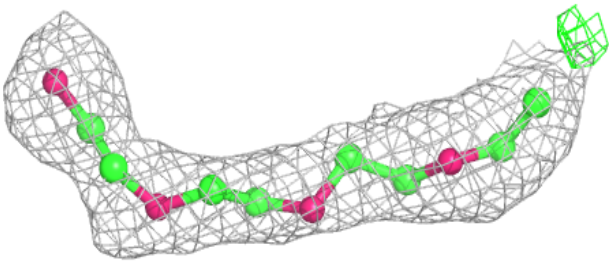


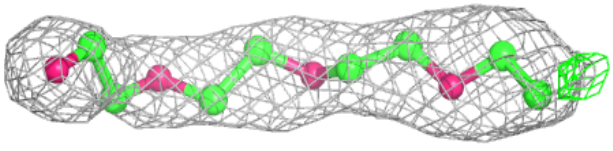


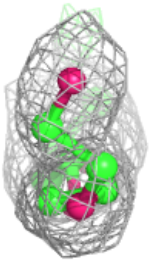


Electron density around C8E C 303:

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

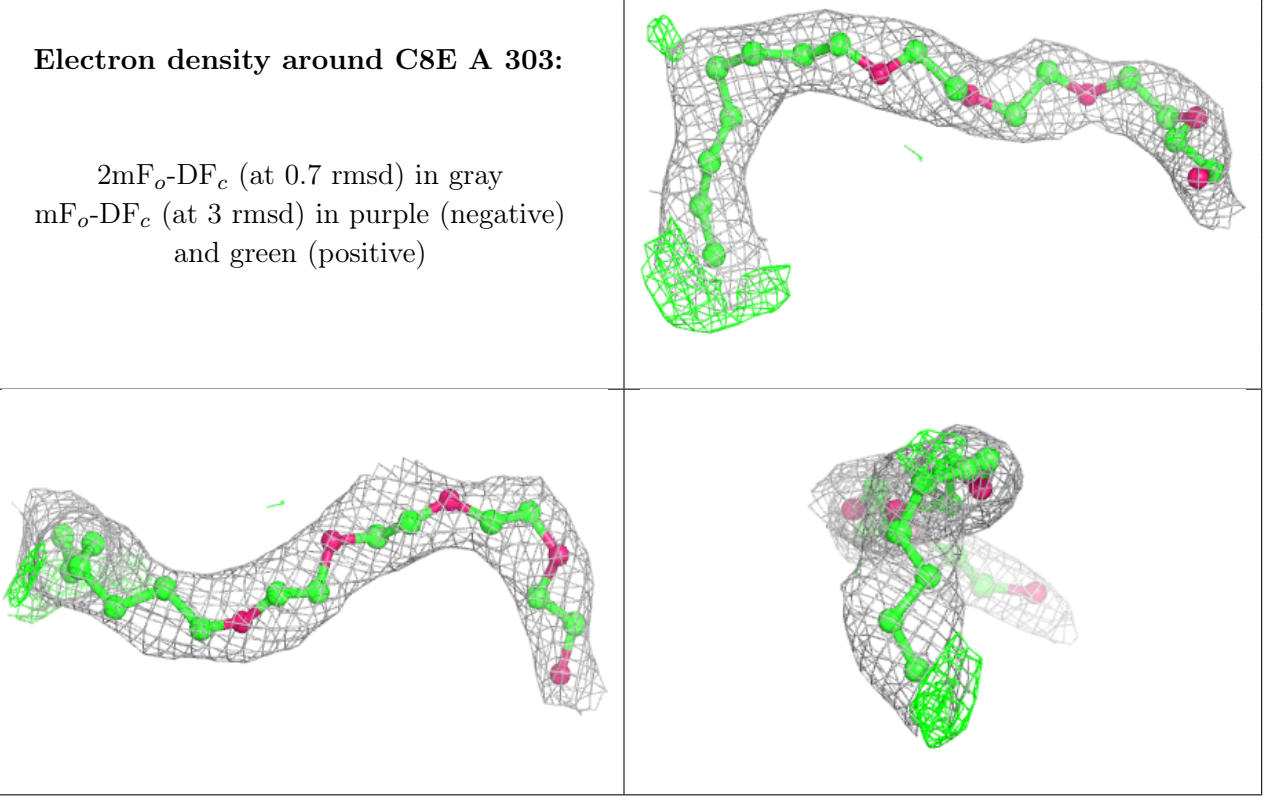






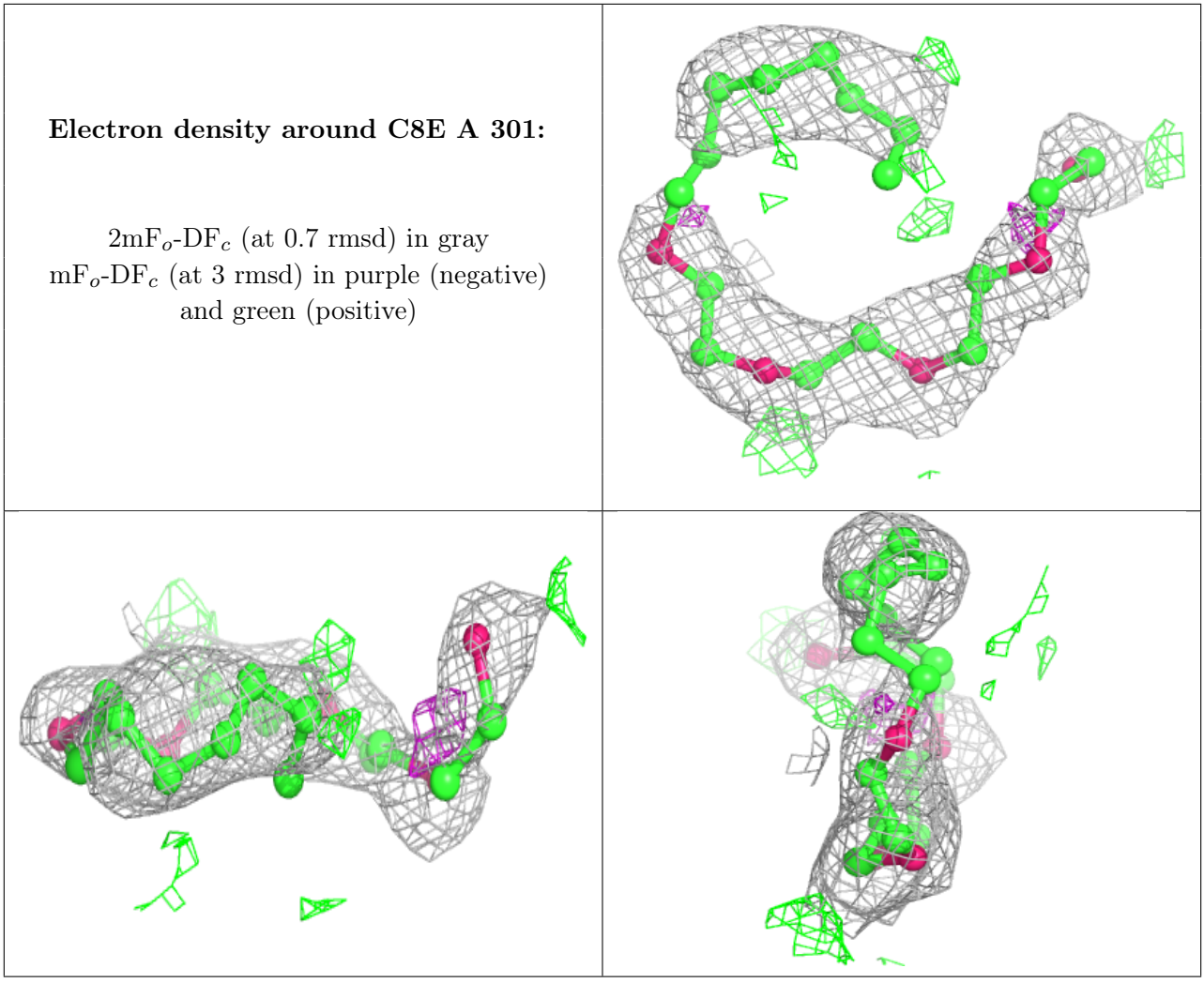
Electron density around C8E A 303:

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



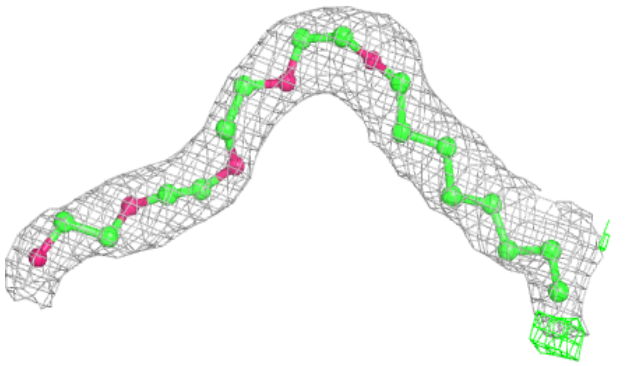
Electron density around C8E A 301:

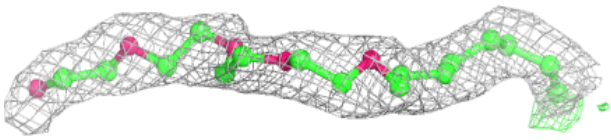
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

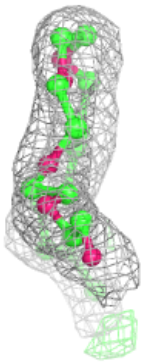


Electron density around C8E B 306:

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

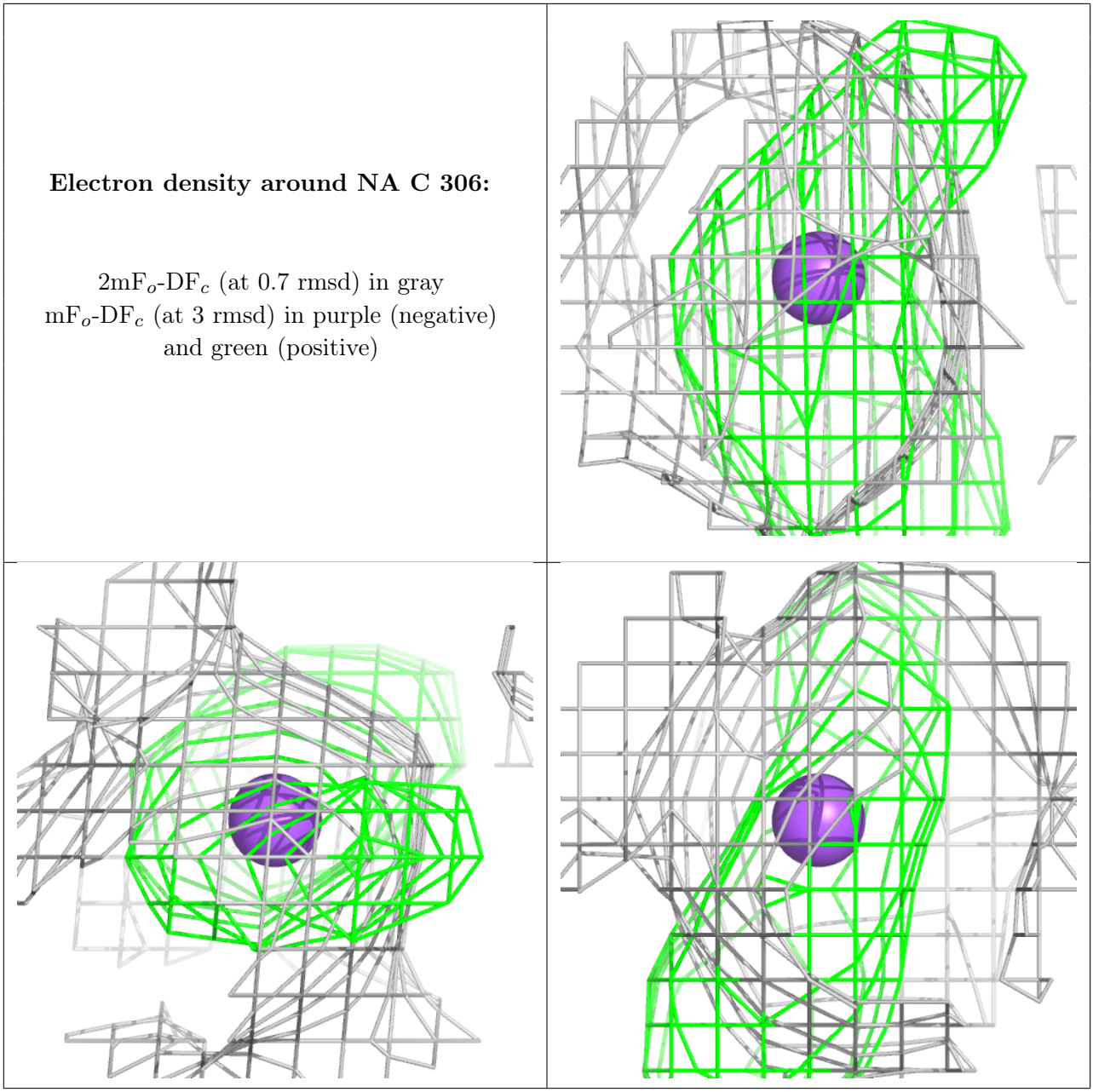






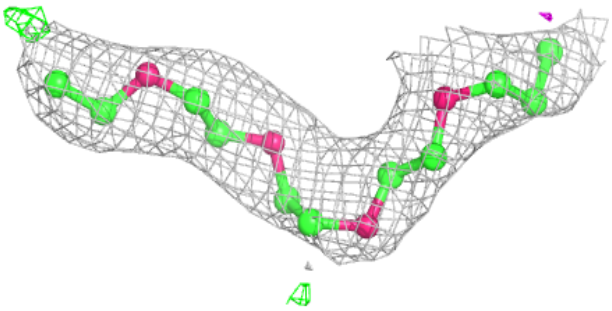
Electron density around NA C 306:

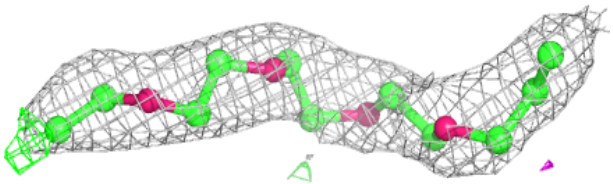
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

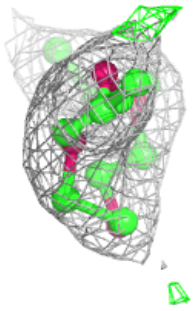


Electron density around C8E A 305:

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

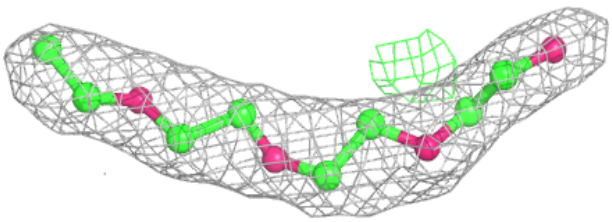


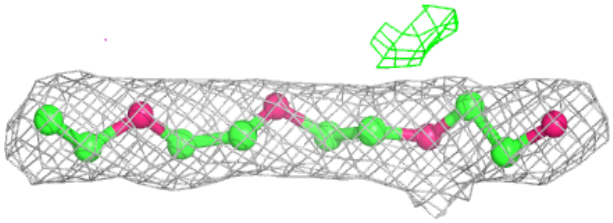


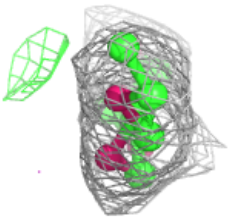


Electron density around C8E A 304:

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

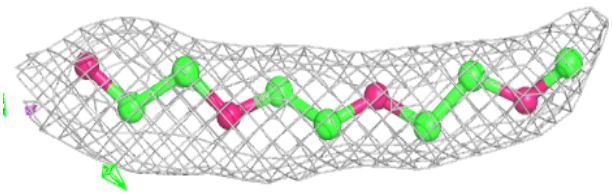


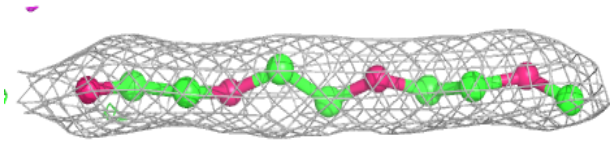


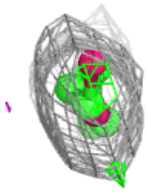


Electron density around C8E B 307:

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

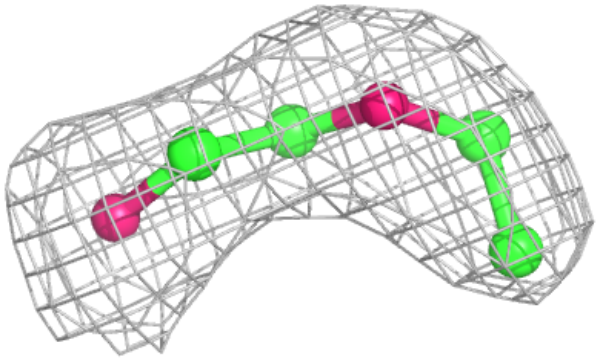


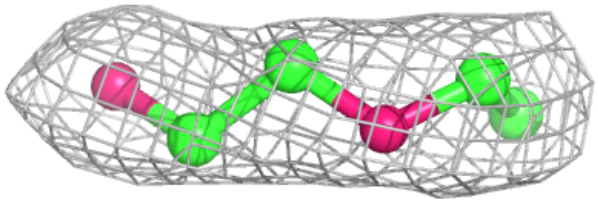


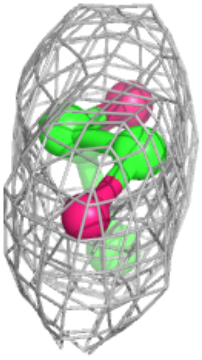


Electron density around C8E D 301:

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

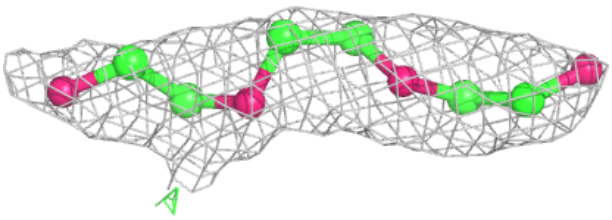


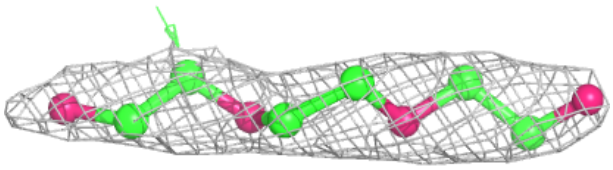


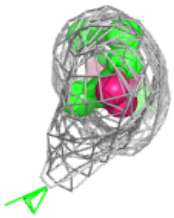


Electron density around C8E C 304:

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

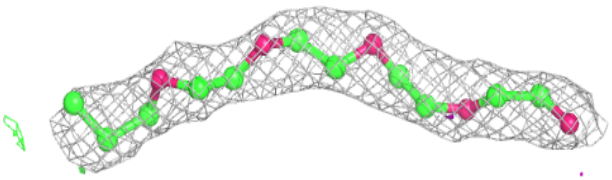


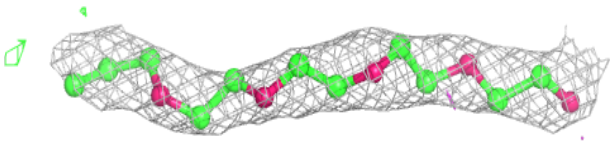


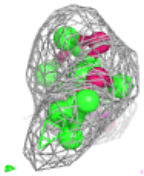


Electron density around C8E C 301:

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

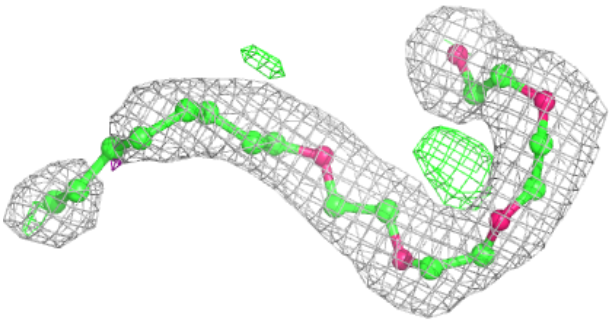


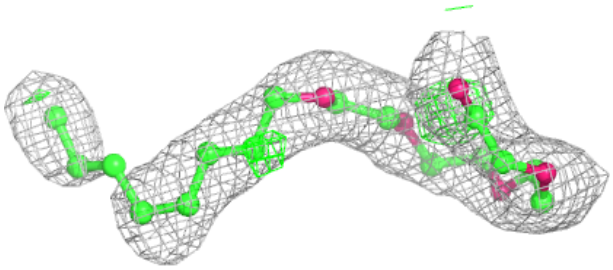


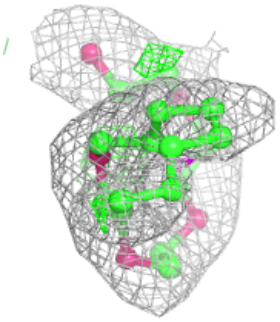


Electron density around C8E B 301:

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

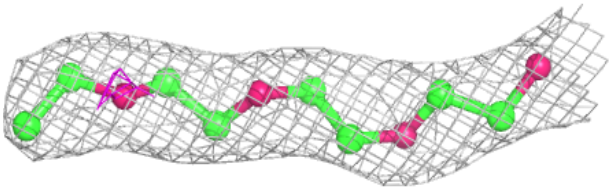


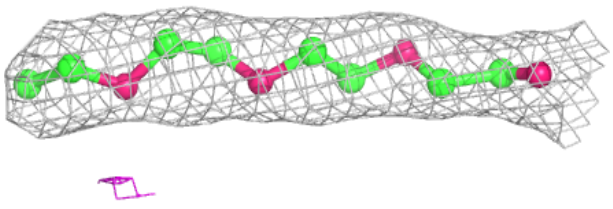


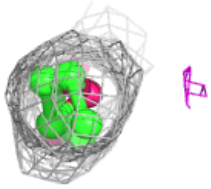


Electron density around C8E B 302:

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

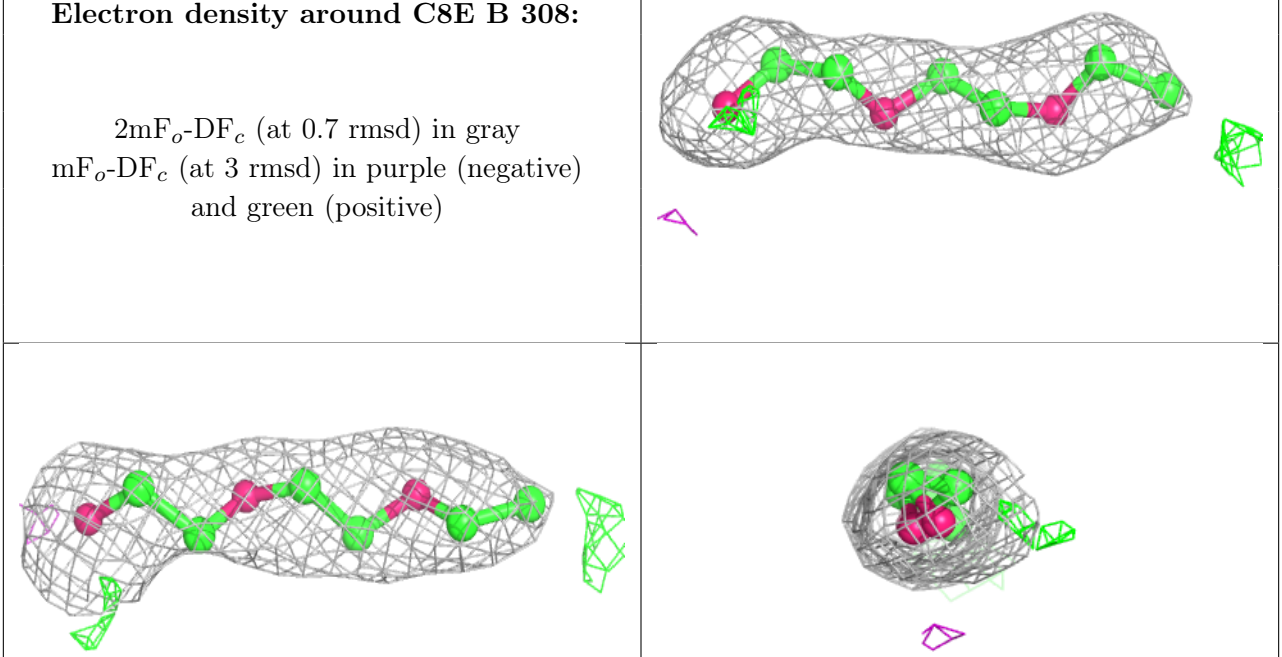






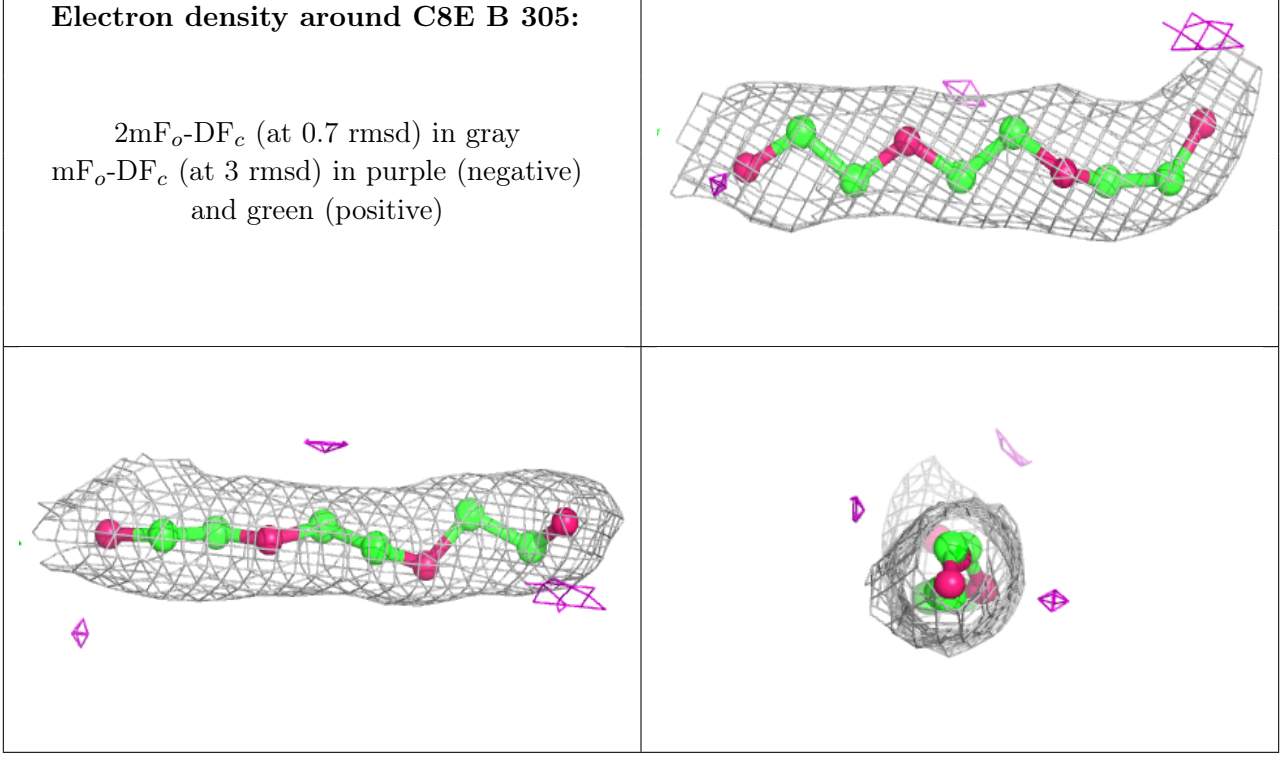
Electron density around C8E B 308:

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



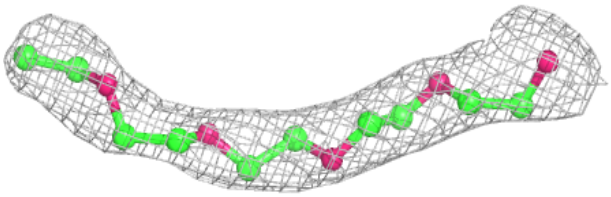
Electron density around C8E B 305:

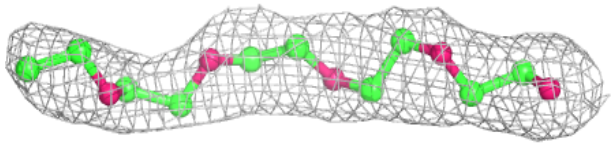
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

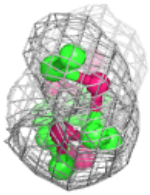


Electron density around C8E A 302:

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

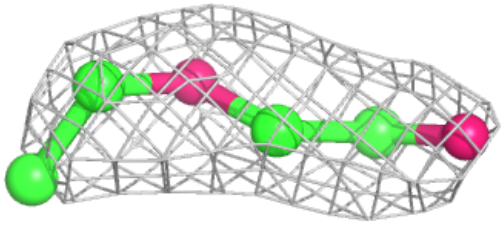


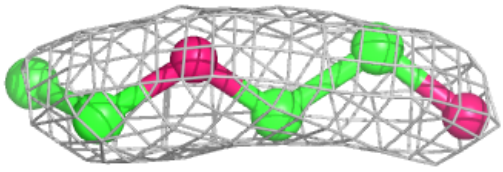


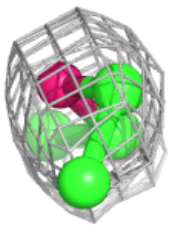


Electron density around C8E C 302:

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

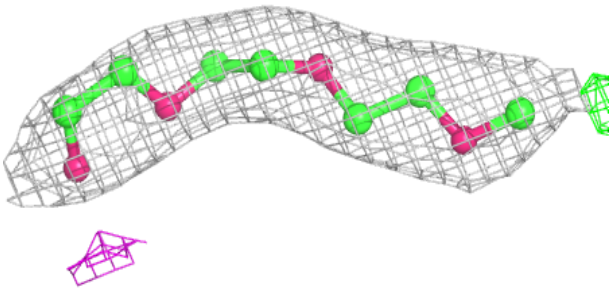


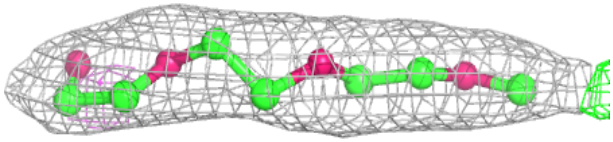


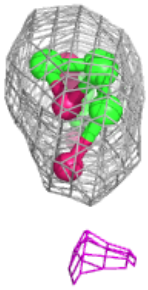


Electron density around C8E B 304:

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

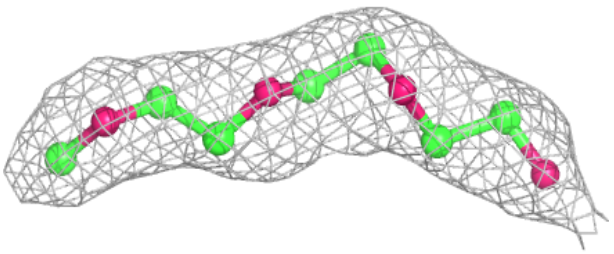


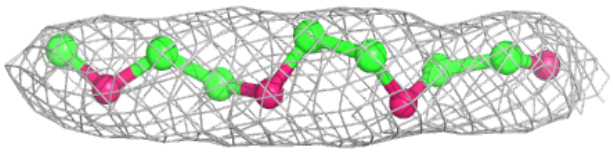


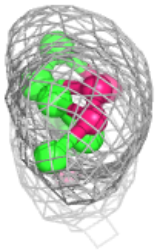


Electron density around C8E B 303:

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

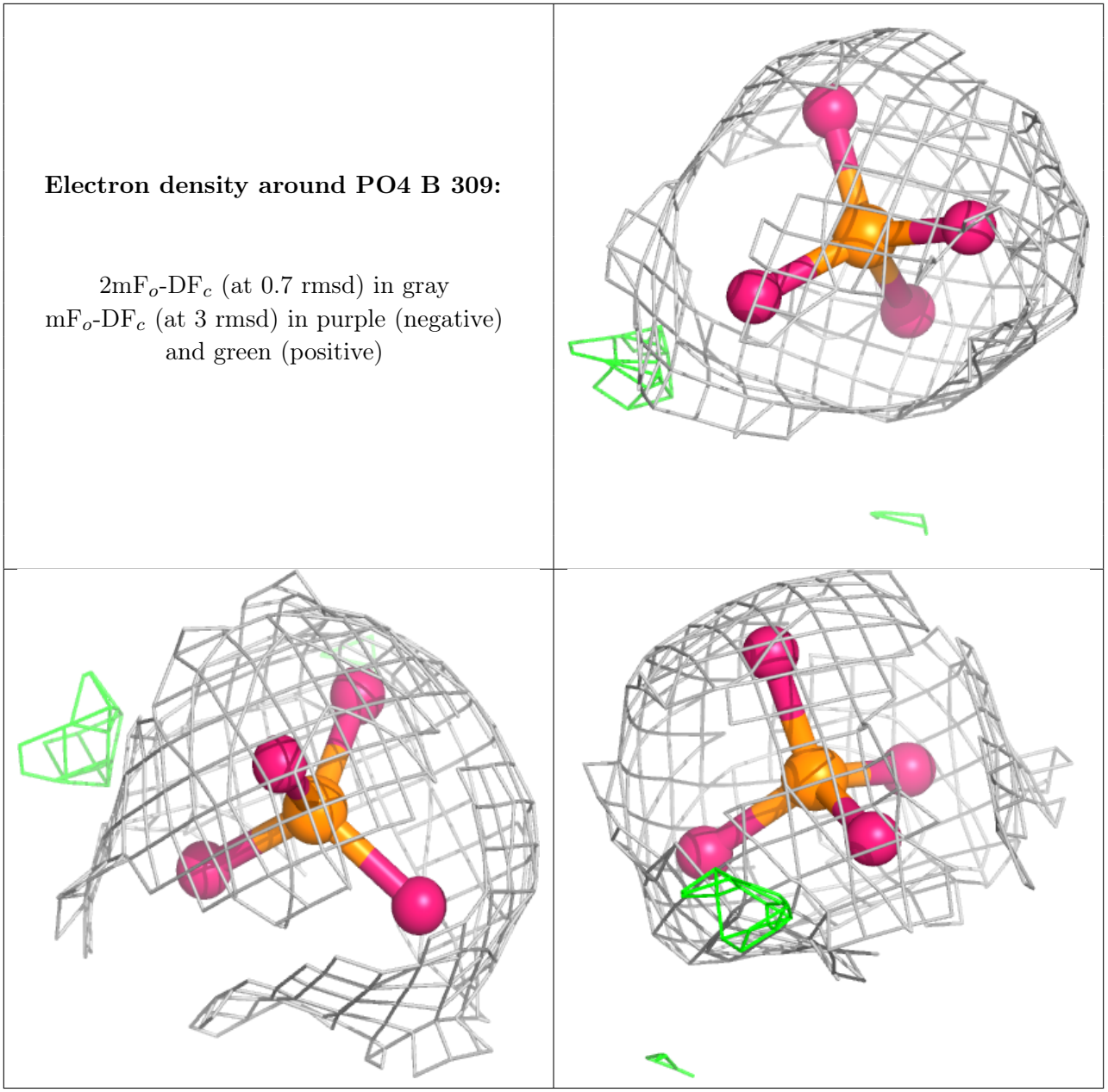






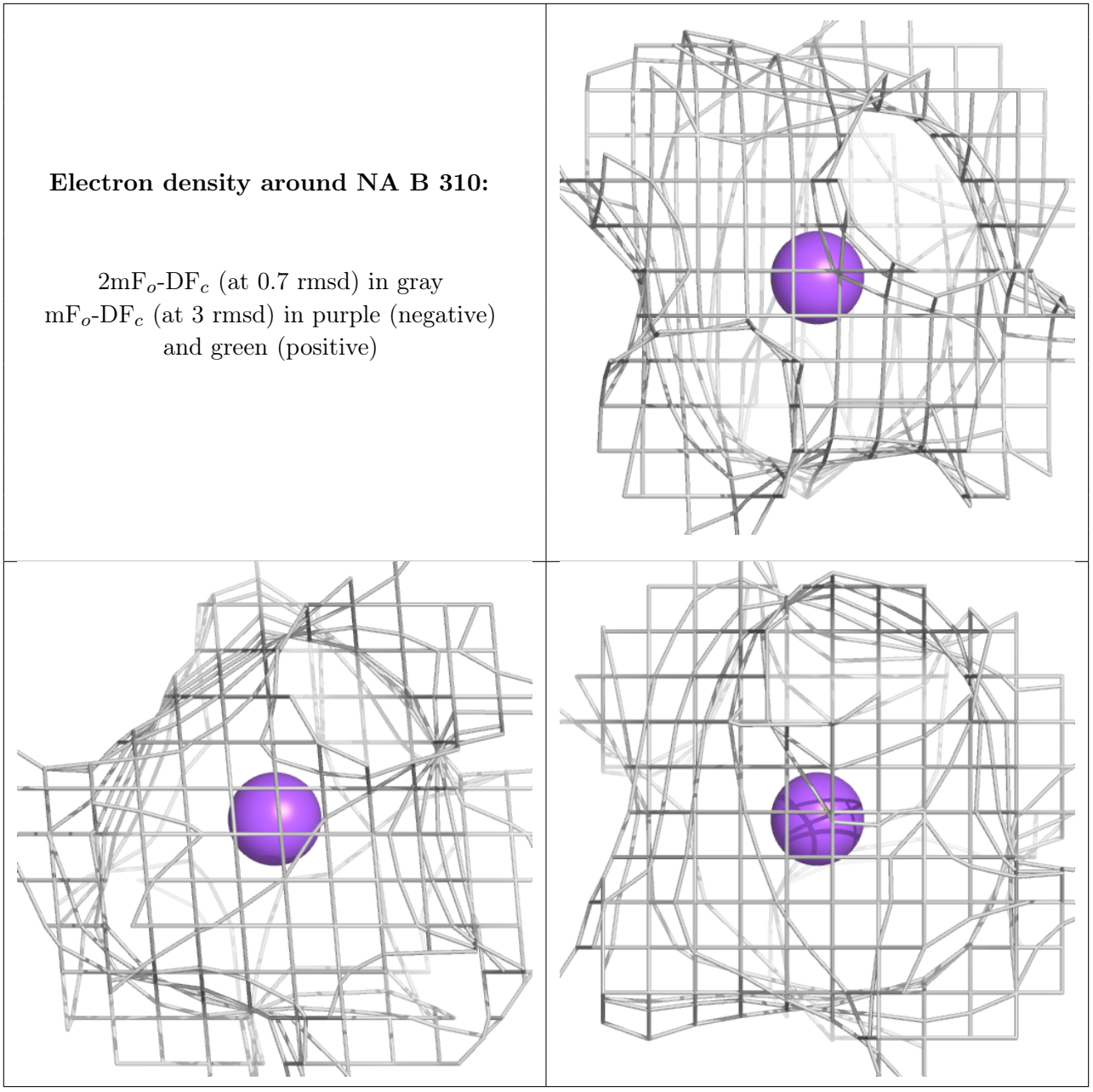
Electron density around PO4 B 309:

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



Electron density around NA B 310:

$2mF_o$-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.