



Full wwPDB X-ray Structure Validation Report i

Apr 28, 2021 – 07:11 pm BST

PDB ID : 6ZHV
Title : Crystal structure of OmpF porin soaked in ciprofloxacin metaloantibiotic
Authors : Sousa, C.F.; Morais-Cabral, J.; Gameiro, P.
Deposited on : 2020-06-23
Resolution : 1.95 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 following versions of software and data (see [references](#) ①) 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	:	2.18
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)	:	2.18

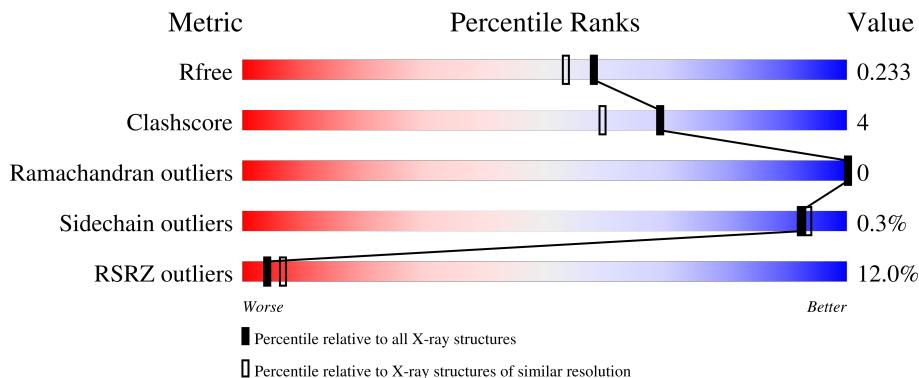
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

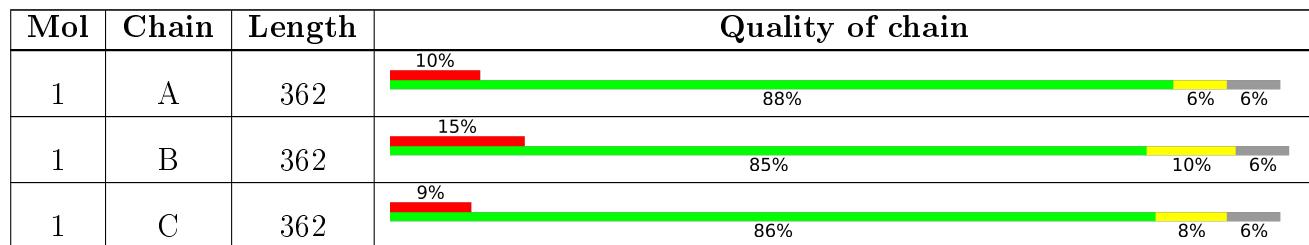
The reported resolution of this entry is 1.95 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition [\(i\)](#)

There are 5 unique types of molecules in this entry. The entry contains 8436 atoms, of which 210 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 Outer membrane porin F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	341	Total	C 2632	N 1657	O 439	S 533	3	0	0
1	A	341	Total	C 2645	N 1666	O 440	S 534	5	0	2
1	C	340	Total	C 2635	N 1659	O 439	S 533	4	0	1

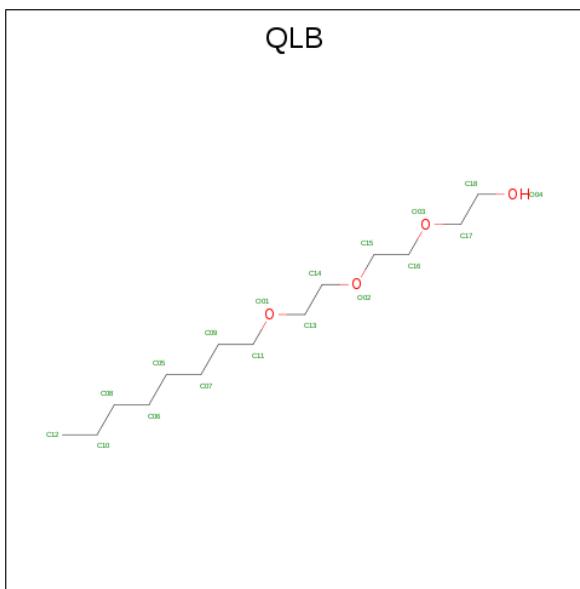
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg 1 1	0	0
2	A	1	Total	Mg 1 1	0	0
2	C	1	Total	Mg 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	Na 5 5	0	0
3	A	4	Total	Na 4 4	0	0
3	C	3	Total	Na 3 3	0	0

- Molecule 4 is 2-[2-(2-octoxyethoxy)ethoxy]ethanol (three-letter code: QLB) (formula: C₁₄H₃₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			48	14	30	4		
4	A	1	Total	C	H	O	0	0
			48	14	30	4		
4	A	1	Total	C	H	O	0	0
			48	14	30	4		
4	C	1	Total	C	H	O	0	0
			48	14	30	4		
4	C	1	Total	C	H	O	0	0
			48	14	30	4		
4	C	1	Total	C	H	O	0	0
			48	14	30	4		

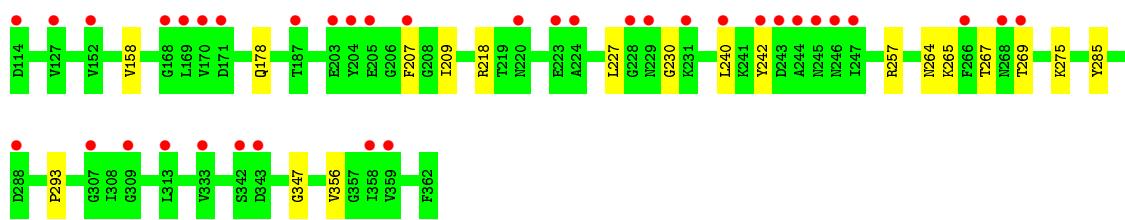
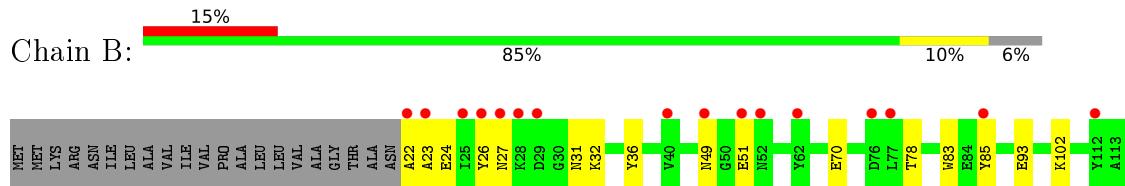
- Molecule 5 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	56	Total	O			0	0
			56	56				
5	A	56	Total	O			0	0
			56	56				
5	C	61	Total	O			0	0
			61	61				

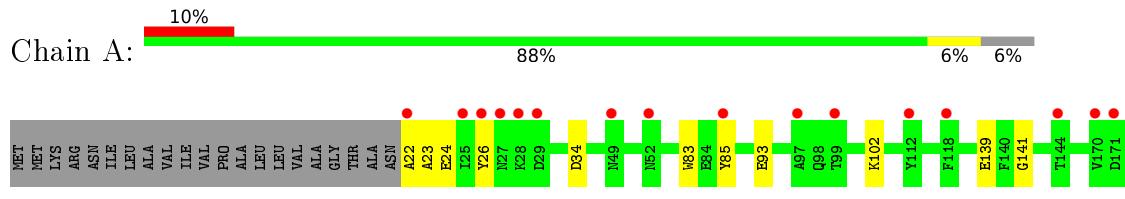
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

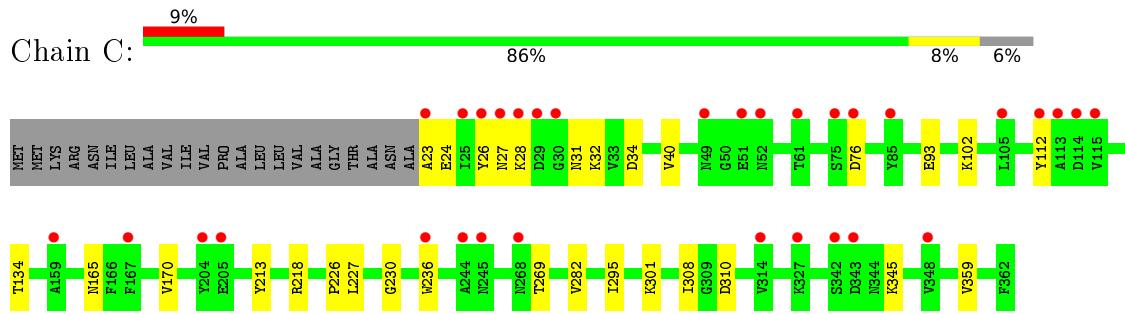
- Molecule 1: Outer membrane porin F



- Molecule 1: Outer membrane porin F



- Molecule 1: Outer membrane porin F



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.03Å 112.00Å 131.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.30 – 1.95 45.68 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.30-1.95) 99.5 (45.68-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.43 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R , R_{free}	0.198 , 0.233 0.198 , 0.233	Depositor DCC
R_{free} test set	4176 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8436	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, QLB, MG

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	0/2704	0.58	0/3655
1	B	0.50	0/2688	0.59	0/3635
1	C	0.50	0/2691	0.60	0/3638
All	All	0.49	0/8083	0.59	0/10928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2462	16	0
1	B	2632	0	2446	25	0
1	C	2635	0	2448	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	3	0	0	0	0
4	A	36	60	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	30	0	2	0
4	C	72	120	0	1	0
5	A	56	0	0	0	0
5	B	56	0	0	0	0
5	C	61	0	0	0	0
All	All	8226	210	7356	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:PRO:HG2	1:C:269:THR:HG23	1.39	1.04
1:A:22:ALA:HB1	1:A:34:ASP:HB3	1.47	0.94
1:B:264:ASN:HB3	1:B:269:THR:HG22	1.63	0.80
1:C:226:PRO:HG2	1:C:269:THR:CG2	2.12	0.80
1:A:22:ALA:HB1	1:A:34:ASP:CB	2.18	0.74
1:C:308:ILE:HG23	1:C:345:LYS:HD2	1.76	0.68
1:A:218:ARG:HD3	1:A:230:GLY:O	1.94	0.67
1:B:49:ASN:HB2	1:B:51:GLU:OE1	1.95	0.67
1:C:24:GLU:HA	1:C:34:ASP:OD1	1.96	0.66
1:C:226:PRO:CG	1:C:269:THR:HG23	2.24	0.64
1:B:70:GLU:HG2	1:B:78:THR:CG2	2.28	0.64
1:B:356:VAL:HG12	4:B:407:QLB:C07	2.30	0.62
1:B:209:ILE:HG22	1:B:240:LEU:CD1	2.30	0.62
1:B:70:GLU:HG2	1:B:78:THR:HG21	1.84	0.60
1:B:26:TYR:HE2	1:B:31:ASN:HB3	1.68	0.59
1:B:27:ASN:HA	1:B:31:ASN:O	2.03	0.58
1:B:207:PHE:CE1	1:B:242:TYR:HB2	2.39	0.57
1:B:22:ALA:N	1:B:36:TYR:HB3	2.20	0.56
1:B:257:ARG:CZ	1:B:275:LYS:HE2	2.36	0.55
1:B:93:GLU:HB3	1:A:102:LYS:HD2	1.89	0.55
1:A:23:ALA:HB1	1:C:26:TYR:HB2	1.88	0.55
1:C:295:ILE:HD12	4:C:408:QLB:C18	2.36	0.55
1:B:209:ILE:HG22	1:B:240:LEU:HD12	1.89	0.54
1:C:76:ASP:HB3	1:C:112:TYR:HE1	1.75	0.52
1:B:26:TYR:HB2	1:C:23:ALA:HB1	1.93	0.50
1:C:227:LEU:HG	1:C:269:THR:HG22	1.93	0.50
1:B:218:ARG:HD3	1:B:230:GLY:O	2.12	0.49
1:A:83:TRP:CZ2	1:A:85:TYR:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ASP:HB3	1:C:112:TYR:CE1	2.48	0.49
1:B:26:TYR:O	1:B:32:LYS:HA	2.15	0.46
1:C:26:TYR:CZ	1:C:28:LYS:HB3	2.51	0.46
1:C:218:ARG:HD3	1:C:230:GLY:O	2.16	0.46
1:B:265:LYS:HD2	1:B:347:GLY:O	2.16	0.45
1:B:23:ALA:HB1	1:A:26:TYR:HB2	1.98	0.45
1:C:40:VAL:HG13	1:C:359:VAL:HG22	1.98	0.45
1:B:102:LYS:HD2	1:C:93:GLU:HB3	1.98	0.45
1:B:267:THR:OG1	1:B:269:THR:HG22	2.16	0.45
1:A:141:GLY:HA2	1:A:316:TYR:OH	2.18	0.44
1:A:256:THR:O	1:A:257:ARG:HD3	2.16	0.43
1:B:227:LEU:HD11	1:B:269:THR:HG23	2.01	0.43
1:A:172:GLY:O	1:A:202:TYR:HA	2.18	0.43
1:C:24:GLU:OE1	1:C:32:LYS:HE2	2.19	0.43
1:A:139:GLU:HB2	1:A:332:TYR:CE1	2.54	0.42
4:B:407:QLB:C18	1:A:179:TYR:HB3	2.50	0.42
1:B:158:VAL:HG22	1:B:178:GLN:CG	2.50	0.42
1:B:285:TYR:O	1:B:293:PRO:HD2	2.20	0.42
1:C:165:ASN:HA	1:C:170:VAL:O	2.20	0.42
1:B:26:TYR:CE2	1:B:31:ASN:HB3	2.50	0.42
1:A:202:TYR:CE2	1:A:204:TYR:HB2	2.54	0.42
1:C:213:TYR:HD2	1:C:236:TRP:HB3	1.84	0.42
1:B:83:TRP:CZ2	1:B:85:TYR:HB2	2.55	0.41
1:C:134:THR:HG22	1:C:282:VAL:HG12	2.01	0.41
1:C:27:ASN:HA	1:C:31:ASN:O	2.21	0.41
1:A:93:GLU:HB3	1:C:102:LYS:HD2	2.02	0.41
1:C:301:LYS:HE3	1:C:310:ASP:HB3	2.03	0.40
1:A:202:TYR:CZ	1:A:204:TYR:HB2	2.55	0.40
1:A:301:LYS:HE2	1:A:312:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	341/362 (94%)	328 (96%)	13 (4%)	0	100	100
1	B	339/362 (94%)	326 (96%)	13 (4%)	0	100	100
1	C	339/362 (94%)	327 (96%)	12 (4%)	0	100	100
All	All	1019/1086 (94%)	981 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/279 (95%)	264 (100%)	1 (0%)	91	91
1	B	263/279 (94%)	262 (100%)	1 (0%)	91	91
1	C	264/279 (95%)	264 (100%)	0	100	100
All	All	792/837 (95%)	790 (100%)	2 (0%)	92	93

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

Mol	Chain	Res	Type
1	B	24	GLU
1	A	24	GLU

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

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 22 ligands modelled in this entry, 15 are monoatomic - leaving 7 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
4	QLB	B	407	-	17,17,17	0.78	0	16,16,16	0.78	1 (6%)
4	QLB	C	406	-	17,17,17	0.73	0	16,16,16	0.60	0
4	QLB	A	407	-	17,17,17	0.73	0	16,16,16	0.66	0
4	QLB	A	406	-	17,17,17	0.79	0	16,16,16	0.76	0
4	QLB	C	407	-	17,17,17	0.71	0	16,16,16	0.57	0
4	QLB	C	405	-	17,17,17	0.68	0	16,16,16	0.55	0
4	QLB	C	408	-	17,17,17	0.73	0	16,16,16	0.65	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
4	QLB	B	407	-	-	5/15/15/15	-
4	QLB	C	406	-	-	8/15/15/15	-
4	QLB	A	407	-	-	6/15/15/15	-
4	QLB	A	406	-	-	10/15/15/15	-
4	QLB	C	407	-	-	8/15/15/15	-
4	QLB	C	405	-	-	6/15/15/15	-
4	QLB	C	408	-	-	5/15/15/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	407	QLB	C07-C05-C06	-2.07	103.90	114.42

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	407	QLB	O01-C13-C14-O02
4	A	406	QLB	C13-C14-O02-C15
4	C	406	QLB	C16-C15-O02-C14
4	A	407	QLB	O01-C13-C14-O02
4	C	407	QLB	O02-C15-C16-O03
4	A	406	QLB	C07-C09-C11-O01
4	B	407	QLB	C07-C09-C11-O01
4	B	407	QLB	O02-C15-C16-O03
4	C	406	QLB	C05-C07-C09-C11
4	C	405	QLB	C05-C07-C09-C11
4	A	407	QLB	O02-C15-C16-O03
4	C	405	QLB	C07-C09-C11-O01
4	C	407	QLB	C07-C09-C11-O01
4	B	407	QLB	C05-C06-C08-C10
4	C	407	QLB	C05-C06-C08-C10
4	A	406	QLB	C05-C06-C08-C10
4	A	406	QLB	O03-C17-C18-O04
4	C	408	QLB	C06-C08-C10-C12
4	A	406	QLB	C14-C13-O01-C11
4	A	406	QLB	C05-C07-C09-C11
4	A	406	QLB	O02-C15-C16-O03
4	C	405	QLB	O02-C15-C16-O03
4	C	405	QLB	O03-C17-C18-O04
4	C	408	QLB	O03-C17-C18-O04
4	C	406	QLB	C09-C11-O01-C13
4	C	407	QLB	C13-C14-O02-C15
4	A	406	QLB	C16-C15-O02-C14
4	C	408	QLB	O01-C13-C14-O02
4	C	406	QLB	O02-C15-C16-O03
4	A	407	QLB	C05-C07-C09-C11
4	A	406	QLB	C06-C08-C10-C12
4	C	405	QLB	C09-C11-O01-C13
4	A	407	QLB	C18-C17-O03-C16
4	C	406	QLB	C13-C14-O02-C15
4	C	406	QLB	C05-C06-C08-C10
4	A	407	QLB	C14-C13-O01-C11
4	C	407	QLB	C16-C15-O02-C14

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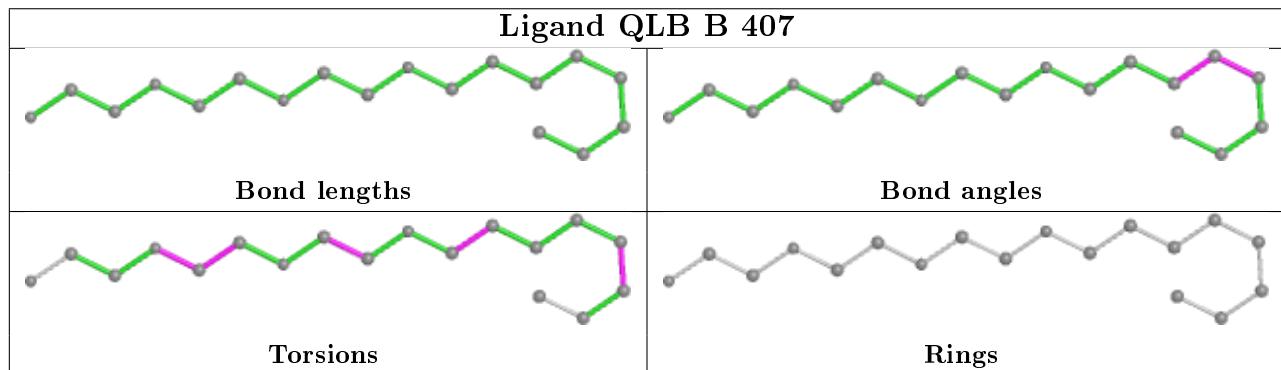
Mol	Chain	Res	Type	Atoms
4	C	407	QLB	C18-C17-O03-C16
4	C	407	QLB	C15-C16-O03-C17
4	C	405	QLB	O01-C13-C14-O02
4	C	407	QLB	O01-C13-C14-O02
4	A	406	QLB	C09-C11-O01-C13
4	C	406	QLB	C18-C17-O03-C16
4	B	407	QLB	C15-C16-O03-C17
4	A	407	QLB	O03-C17-C18-O04
4	C	408	QLB	C09-C11-O01-C13
4	C	406	QLB	C07-C09-C11-O01
4	C	408	QLB	O02-C15-C16-O03

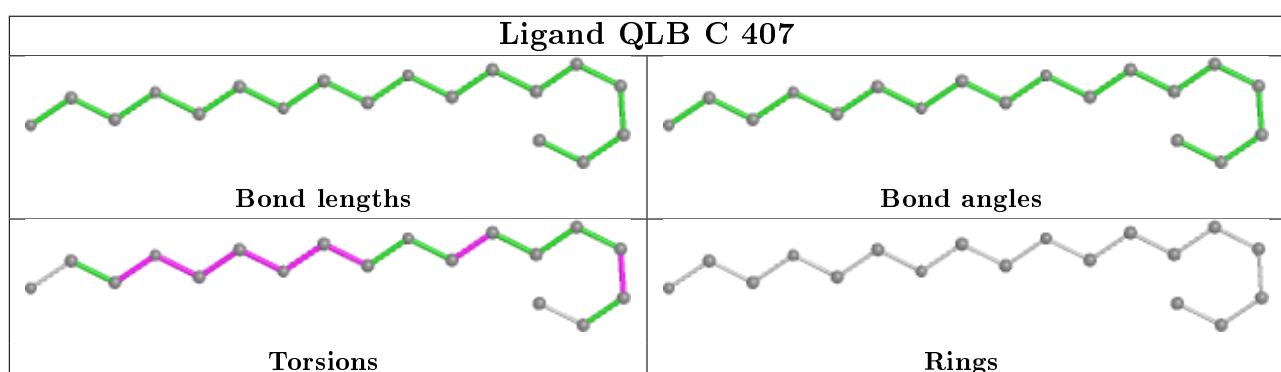
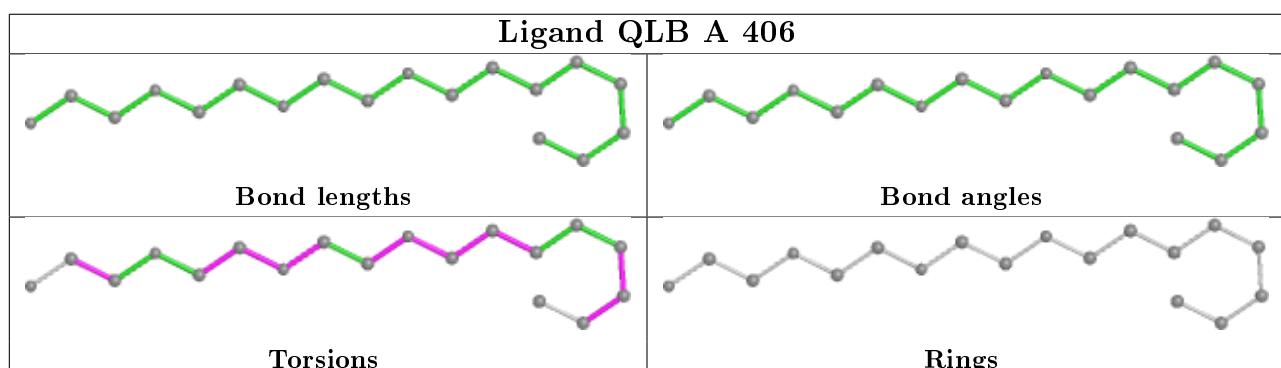
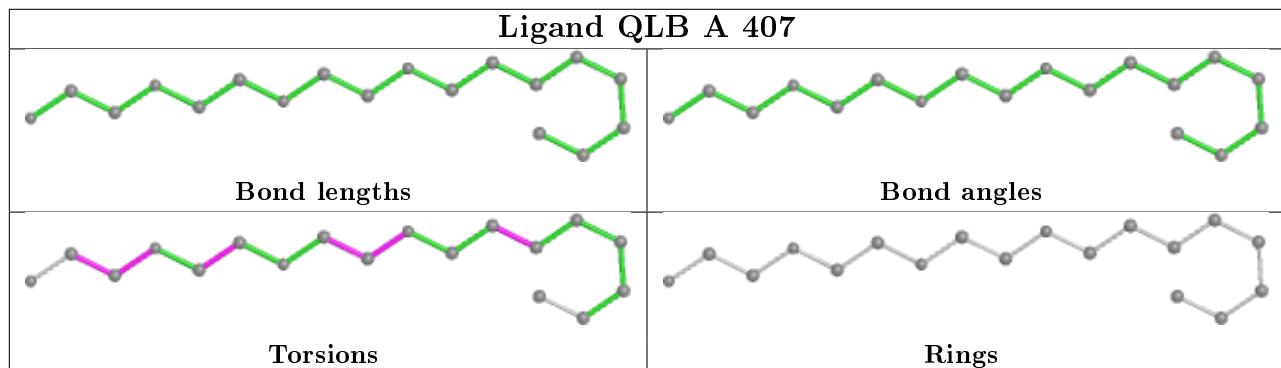
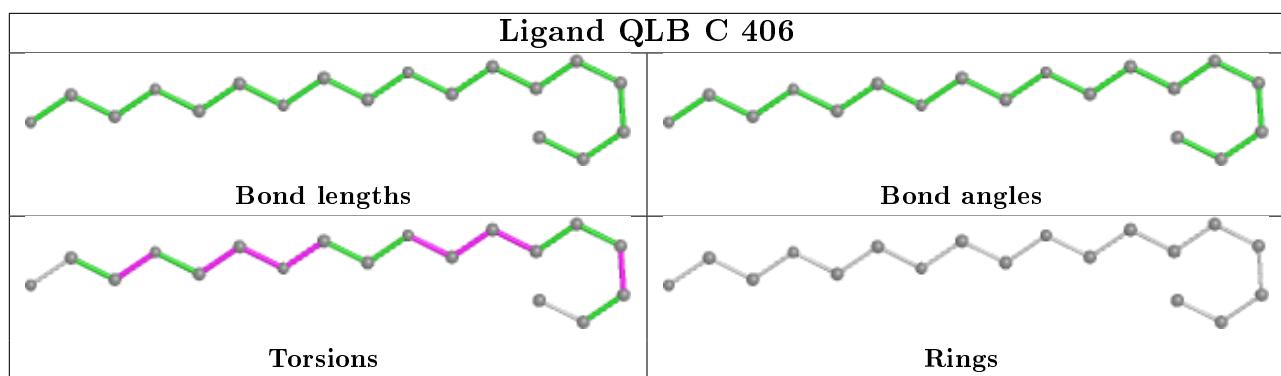
There are no ring outliers.

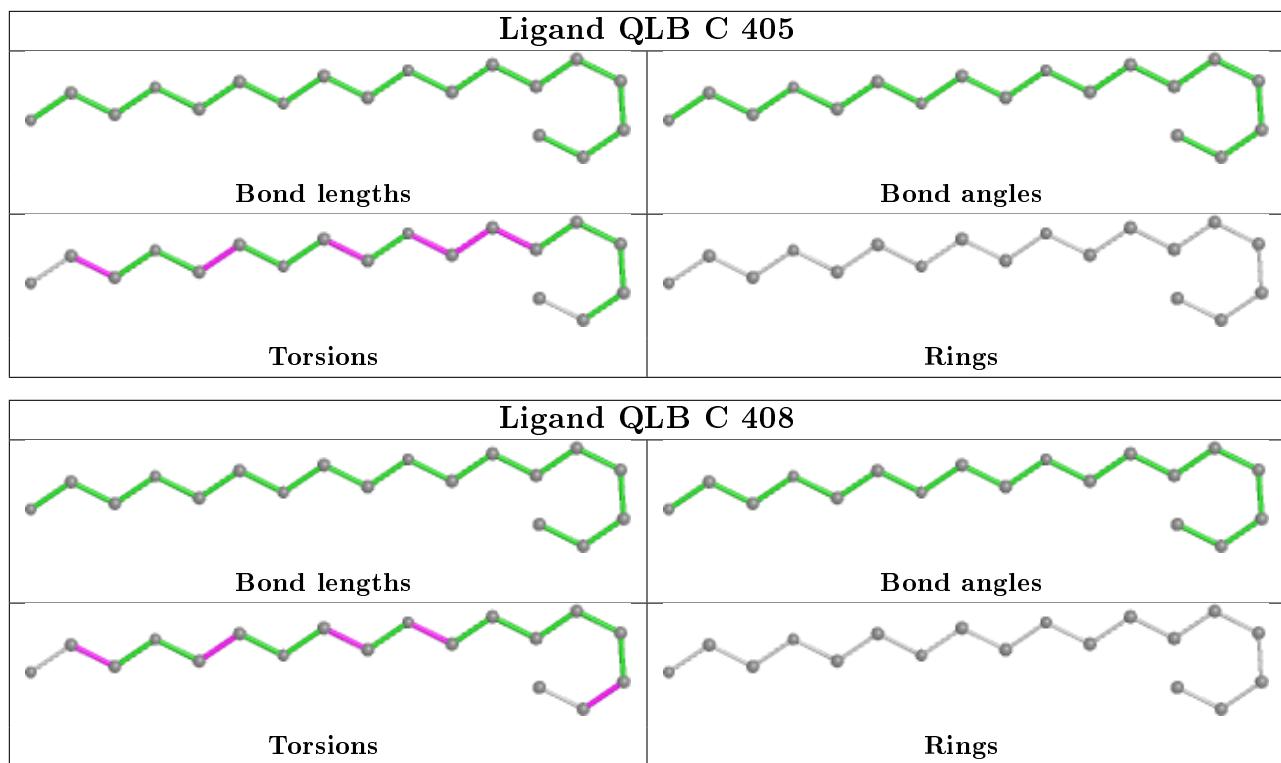
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	407	QLB	2	0
4	C	408	QLB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [\(i\)](#)

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	341/362 (94%)	1.09	38 (11%) 5 8	17, 27, 46, 65	0
1	B	341/362 (94%)	1.20	53 (15%) 2 2	17, 27, 49, 68	0
1	C	340/362 (93%)	1.04	32 (9%) 8 12	16, 26, 46, 68	0
All	All	1022/1086 (94%)	1.11	123 (12%) 4 7	16, 27, 47, 68	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	TYR	10.6
1	B	204	TYR	10.5
1	A	204	TYR	8.8
1	C	28	LYS	8.0
1	A	26	TYR	7.9
1	C	114	ASP	6.8
1	A	22	ALA	6.8
1	A	28	LYS	6.7
1	B	25	ILE	6.6
1	B	28	LYS	6.1
1	A	25	ILE	6.0
1	B	26	TYR	6.0
1	A	205	GLU	5.8
1	C	26	TYR	5.8
1	B	242	TYR	5.8
1	C	115	VAL	5.8
1	A	29	ASP	5.7
1	B	205	GLU	5.7
1	C	30	GLY	5.4
1	A	269	THR	5.4
1	B	207	PHE	5.4
1	B	244	ALA	5.3
1	B	29	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	25	ILE	4.8
1	B	27	ASN	4.7
1	C	29	ASP	4.6
1	C	27	ASN	4.5
1	A	229	ASN	4.4
1	C	342	SER	4.4
1	B	168	GLY	4.3
1	B	268	ASN	4.2
1	C	245	ASN	4.1
1	B	49	ASN	4.1
1	B	169	LEU	4.0
1	B	269	THR	3.7
1	C	112	TYR	3.6
1	A	27	ASN	3.6
1	B	245	ASN	3.6
1	B	170	VAL	3.5
1	A	112	TYR	3.4
1	C	51	GLU	3.3
1	B	22	ALA	3.3
1	B	23	ALA	3.2
1	C	268	ASN	3.2
1	C	343	ASP	3.2
1	A	49	ASN	3.1
1	A	207	PHE	3.1
1	B	224	ALA	3.0
1	B	171	ASP	3.0
1	B	343	ASP	3.0
1	B	246	ASN	3.0
1	A	288	ASP	3.0
1	A	223	GLU	2.9
1	B	112	TYR	2.9
1	C	113	ALA	2.8
1	B	114	ASP	2.7
1	B	85	TYR	2.7
1	B	223	GLU	2.7
1	B	76	ASP	2.7
1	B	307	GLY	2.6
1	C	76	ASP	2.6
1	A	85	TYR	2.6
1	A	253	TYR	2.6
1	A	206	GLY	2.6
1	B	266	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	2.5
1	C	75	SER	2.5
1	C	85	TYR	2.5
1	A	354	VAL	2.5
1	C	348	VAL	2.5
1	B	243	ASP	2.4
1	A	266	PHE	2.4
1	B	40	VAL	2.4
1	A	186	ASP	2.4
1	A	309	GLY	2.4
1	B	231	LYS	2.4
1	A	308	ILE	2.4
1	C	49	ASN	2.4
1	C	236	TRP	2.4
1	A	327	LYS	2.4
1	B	247	ILE	2.4
1	A	97	ALA	2.3
1	B	203	GLU	2.3
1	C	167	PHE	2.3
1	B	309	GLY	2.3
1	C	314	VAL	2.3
1	B	62	TYR	2.3
1	A	347	GLY	2.3
1	C	159	ALA	2.3
1	B	342	SER	2.3
1	B	127	VAL	2.3
1	C	23	ALA	2.3
1	C	205	GLU	2.2
1	A	242	TYR	2.2
1	B	52	ASN	2.2
1	B	229	ASN	2.2
1	A	343	ASP	2.2
1	B	77	LEU	2.2
1	B	240	LEU	2.2
1	C	105	LEU	2.2
1	A	118	PHE	2.2
1	B	228	GLY	2.2
1	B	358	ILE	2.2
1	A	52	ASN	2.2
1	B	187	THR	2.1
1	C	52	ASN	2.1
1	B	152	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	THR	2.1
1	A	270	SER	2.1
1	A	170	VAL	2.1
1	C	61	THR	2.1
1	B	333	VAL	2.1
1	A	287	PHE	2.1
1	C	244	ALA	2.1
1	A	99	THR	2.0
1	A	267	THR	2.0
1	B	51	GLU	2.0
1	B	359	VAL	2.0
1	B	220	ASN	2.0
1	B	288	ASP	2.0
1	A	171	ASP	2.0
1	B	313	LEU	2.0
1	C	327	LYS	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.

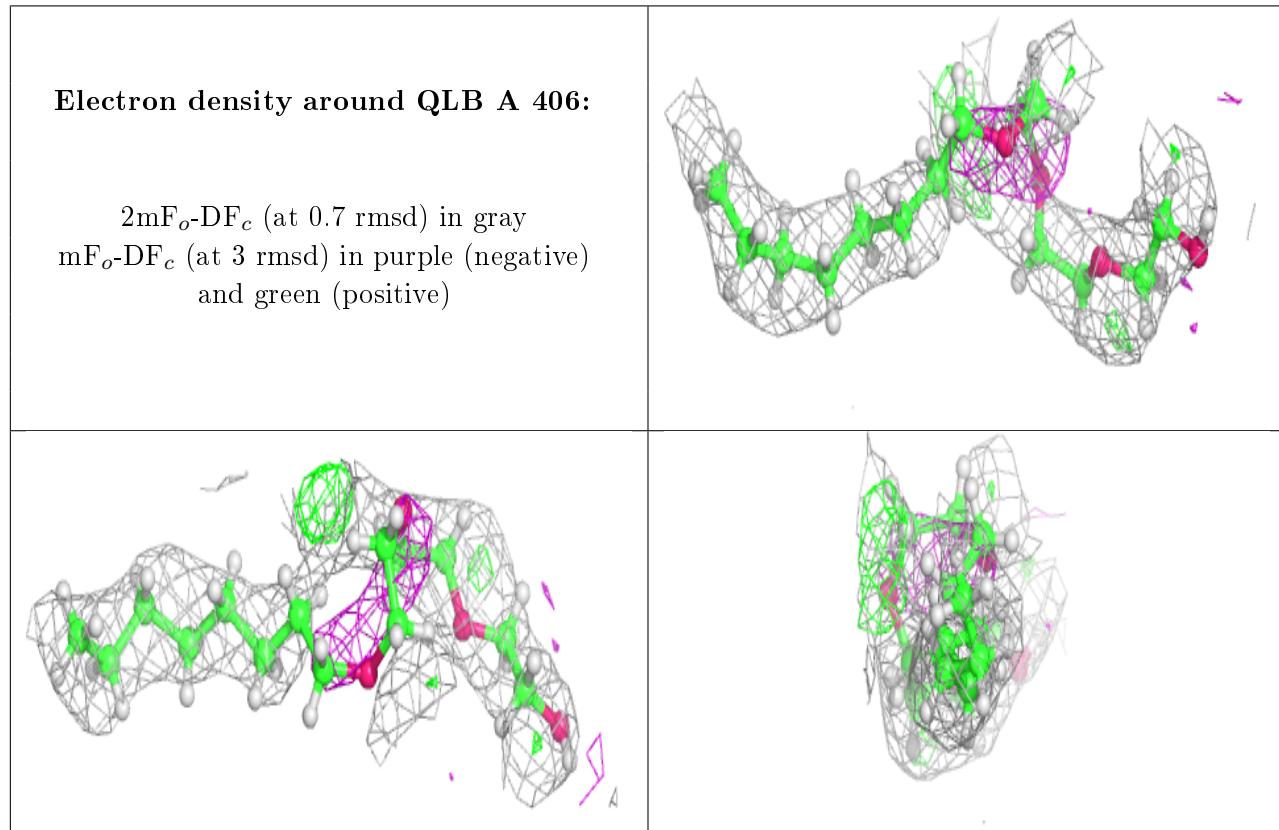
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QLB	A	406	18/18	0.58	0.34	33,46,78,85	0
4	QLB	C	407	18/18	0.60	0.25	34,51,74,87	0
4	QLB	C	406	18/18	0.61	0.35	40,62,78,88	0
4	QLB	B	407	18/18	0.61	0.27	36,48,63,63	0
4	QLB	A	407	18/18	0.69	0.26	35,45,69,69	0
4	QLB	C	408	18/18	0.72	0.30	36,53,89,92	0
4	QLB	C	405	18/18	0.80	0.20	32,47,65,67	0

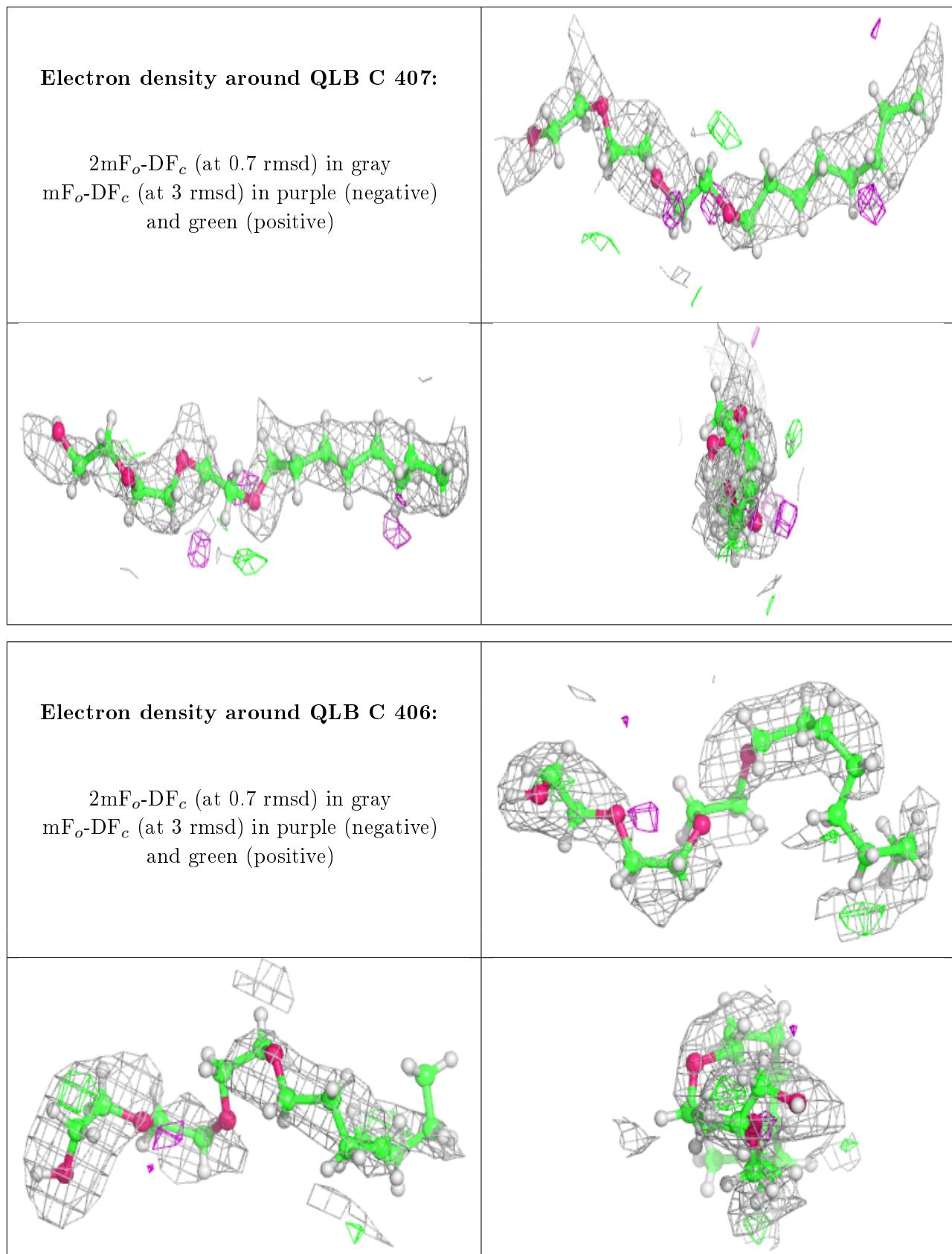
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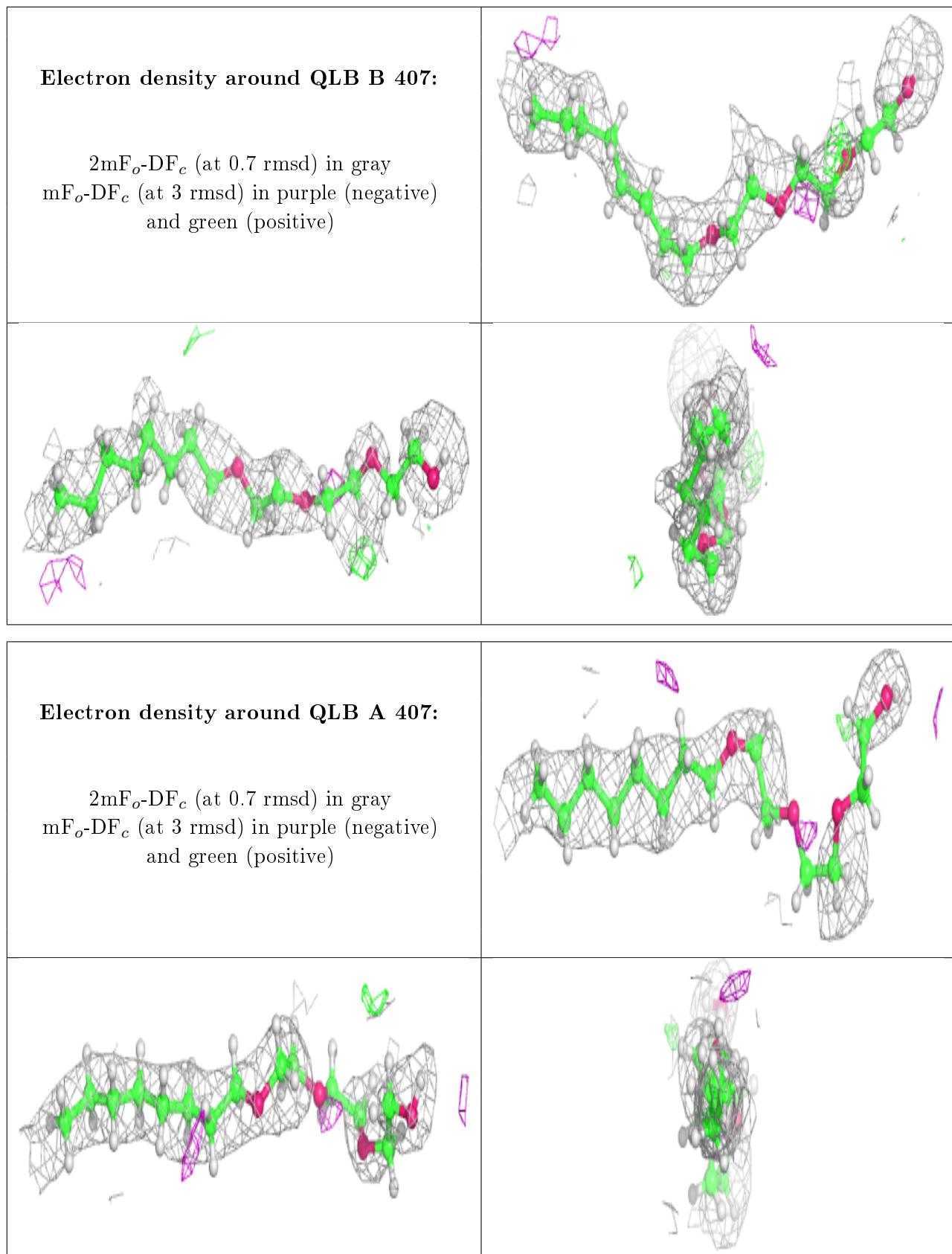
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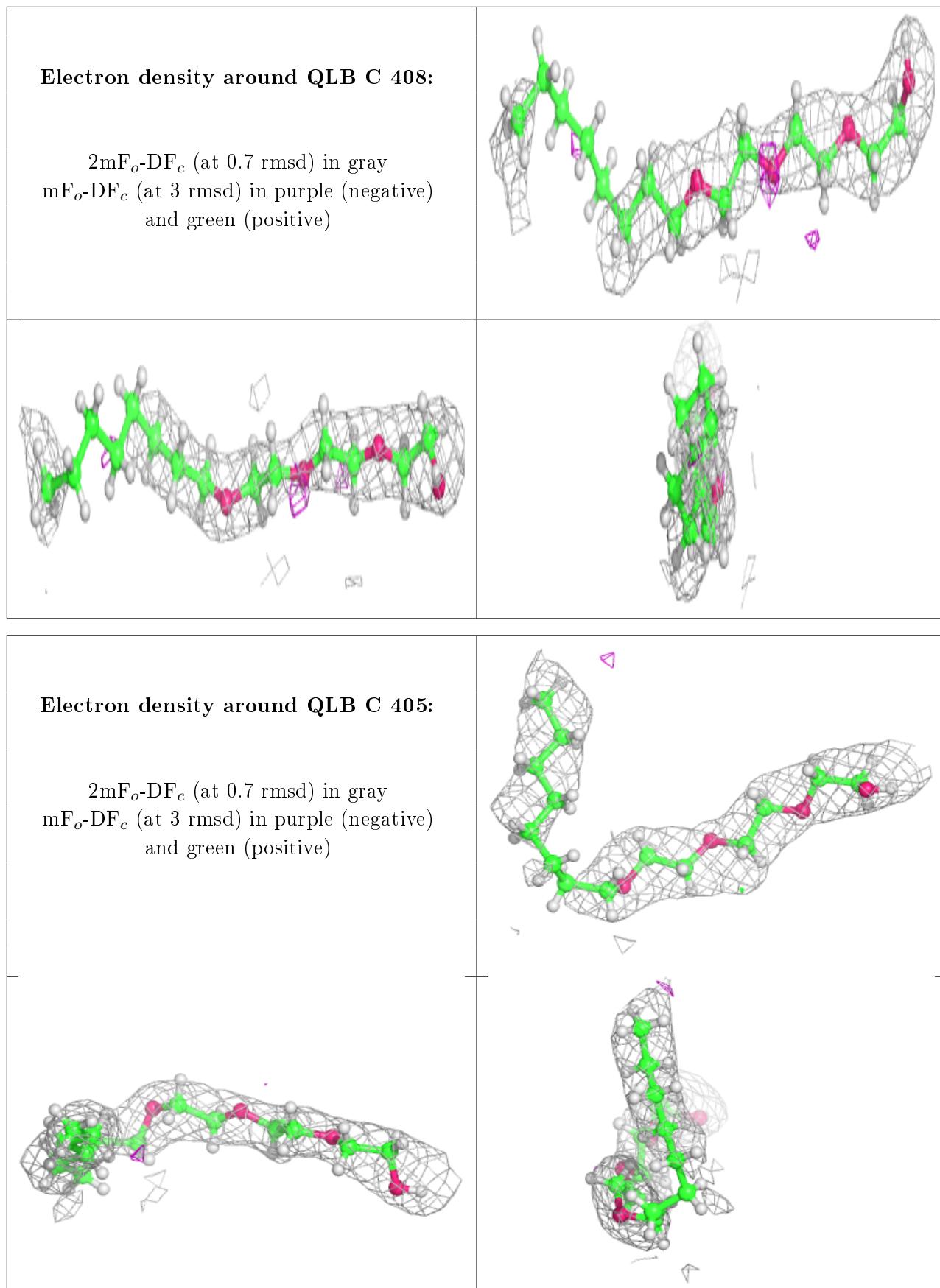
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	C	402	1/1	0.80	0.13	34,34,34,34	0
3	NA	C	404	1/1	0.81	0.15	36,36,36,36	0
3	NA	B	404	1/1	0.83	0.11	39,39,39,39	0
3	NA	B	405	1/1	0.84	0.34	45,45,45,45	0
3	NA	C	403	1/1	0.88	0.27	50,50,50,50	0
3	NA	B	402	1/1	0.89	0.20	35,35,35,35	0
2	MG	A	401	1/1	0.90	0.20	36,36,36,36	0
3	NA	A	402	1/1	0.91	0.46	46,46,46,46	0
3	NA	A	403	1/1	0.91	0.08	44,44,44,44	0
2	MG	C	401	1/1	0.91	0.16	30,30,30,30	0
3	NA	A	404	1/1	0.93	0.18	37,37,37,37	0
2	MG	B	401	1/1	0.94	0.08	32,32,32,32	0
3	NA	A	405	1/1	0.94	0.23	43,43,43,43	0
3	NA	B	403	1/1	0.94	0.32	44,44,44,44	0
3	NA	B	406	1/1	0.95	0.29	44,44,44,44	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.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.