



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:52 am GMT

PDB ID : 6GR0
Title : Petrobactin-binding engineered lipocalin in complex with gallium-petrobactin
Authors : Skerra, A.; Eichinger, A.
Deposited on : 2018-06-08
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

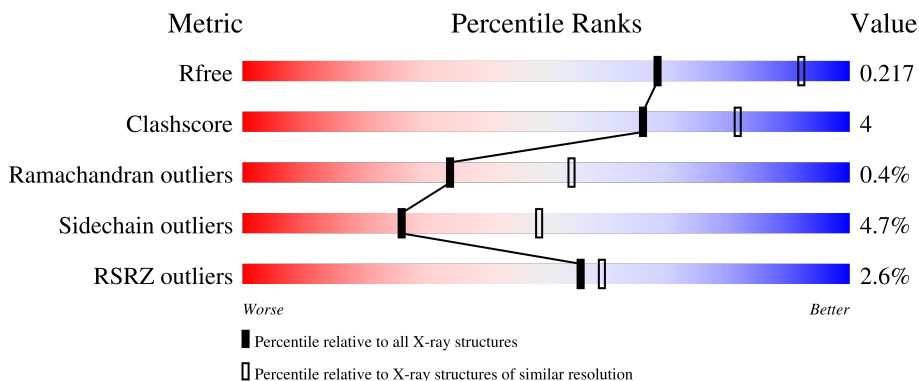
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


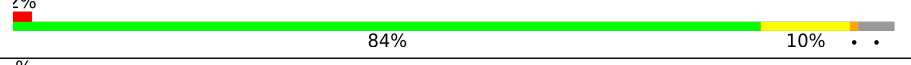

The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	174	 5% 86% 10% . .
1	B	174	 2% 84% 10% . .
1	C	174	 % 89% 6% . 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4570 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 Neutrophil gelatinase-associated lipocalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1415	911	238	261	5	0	0	0
1	B	167	1361	881	227	248	5	0	0	0
1	C	166	1353	875	226	247	5	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	HIS	GLN	engineered mutation	UNP P80188
A	36	PHE	LEU	engineered mutation	UNP P80188
A	38	GLU	GLY	engineered mutation	UNP P80188
A	40	ILE	ALA	engineered mutation	UNP P80188
A	41	GLN	ILE	engineered mutation	UNP P80188
A	42	GLN	LEU	engineered mutation	UNP P80188
A	49	PRO	GLN	engineered mutation	UNP P80188
A	52	ILE	TYR	engineered mutation	UNP P80188
A	68	ASN	SER	engineered mutation	UNP P80188
A	70	ALA	LEU	engineered mutation	UNP P80188
A	71	SER	PHE	engineered mutation	UNP P80188
A	72	ASN	ARG	engineered mutation	UNP P80188
A	73	TRP	LYS	engineered mutation	UNP P80188
A	74	GLU	LYS	engineered mutation	UNP P80188
A	77	THR	ASP	engineered mutation	UNP P80188
A	79	ARG	TRP	engineered mutation	UNP P80188
A	81	LYS	ARG	engineered mutation	UNP P80188
A	87	SER	CYS	engineered mutation	UNP P80188
A	96	GLU	ASN	engineered mutation	UNP P80188
A	100	ARG	TYR	engineered mutation	UNP P80188
A	103	MET	LEU	engineered mutation	UNP P80188
A	125	THR	LYS	engineered mutation	UNP P80188
A	127	VAL	SER	engineered mutation	UNP P80188

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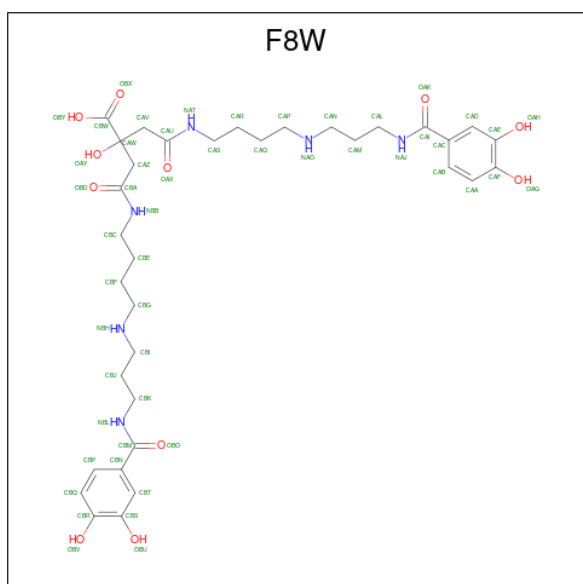
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LYS	TYR	engineered mutation	UNP P80188
A	134	TRP	LYS	engineered mutation	UNP P80188
B	28	HIS	GLN	engineered mutation	UNP P80188
B	36	PHE	LEU	engineered mutation	UNP P80188
B	38	GLU	GLY	engineered mutation	UNP P80188
B	40	ILE	ALA	engineered mutation	UNP P80188
B	41	GLN	ILE	engineered mutation	UNP P80188
B	42	GLN	LEU	engineered mutation	UNP P80188
B	49	PRO	GLN	engineered mutation	UNP P80188
B	52	ILE	TYR	engineered mutation	UNP P80188
B	68	ASN	SER	engineered mutation	UNP P80188
B	70	ALA	LEU	engineered mutation	UNP P80188
B	71	SER	PHE	engineered mutation	UNP P80188
B	72	ASN	ARG	engineered mutation	UNP P80188
B	73	TRP	LYS	engineered mutation	UNP P80188
B	74	GLU	LYS	engineered mutation	UNP P80188
B	77	THR	ASP	engineered mutation	UNP P80188
B	79	ARG	TRP	engineered mutation	UNP P80188
B	81	LYS	ARG	engineered mutation	UNP P80188
B	87	SER	CYS	engineered mutation	UNP P80188
B	96	GLU	ASN	engineered mutation	UNP P80188
B	100	ARG	TYR	engineered mutation	UNP P80188
B	103	MET	LEU	engineered mutation	UNP P80188
B	125	THR	LYS	engineered mutation	UNP P80188
B	127	VAL	SER	engineered mutation	UNP P80188
B	132	LYS	TYR	engineered mutation	UNP P80188
B	134	TRP	LYS	engineered mutation	UNP P80188
C	28	HIS	GLN	engineered mutation	UNP P80188
C	36	PHE	LEU	engineered mutation	UNP P80188
C	38	GLU	GLY	engineered mutation	UNP P80188
C	40	ILE	ALA	engineered mutation	UNP P80188
C	41	GLN	ILE	engineered mutation	UNP P80188
C	42	GLN	LEU	engineered mutation	UNP P80188
C	49	PRO	GLN	engineered mutation	UNP P80188
C	52	ILE	TYR	engineered mutation	UNP P80188
C	68	ASN	SER	engineered mutation	UNP P80188
C	70	ALA	LEU	engineered mutation	UNP P80188
C	71	SER	PHE	engineered mutation	UNP P80188
C	72	ASN	ARG	engineered mutation	UNP P80188
C	73	TRP	LYS	engineered mutation	UNP P80188
C	74	GLU	LYS	engineered mutation	UNP P80188
C	77	THR	ASP	engineered mutation	UNP P80188

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Chain	Residue	Modelled	Actual	Comment	Reference
C	79	ARG	TRP	engineered mutation	UNP P80188
C	81	LYS	ARG	engineered mutation	UNP P80188
C	87	SER	CYS	engineered mutation	UNP P80188
C	96	GLU	ASN	engineered mutation	UNP P80188
C	100	ARG	TYR	engineered mutation	UNP P80188
C	103	MET	LEU	engineered mutation	UNP P80188
C	125	THR	LYS	engineered mutation	UNP P80188
C	127	VAL	SER	engineered mutation	UNP P80188
C	132	LYS	TYR	engineered mutation	UNP P80188
C	134	TRP	LYS	engineered mutation	UNP P80188

- Molecule 2 is 4-[4-[3-[[3,4-bis(oxidanyl)phenyl]carbonylamino]propylamino]butylamino]-2-[2-[4-[3-[[3,4-bis(oxidanyl)phenyl]carbonylamino]propylamino]butylamino]-2-oxidanylidene-ethyl]-2-oxidanyl-4-oxidanylidene-butanoic acid (three-letter code: F8W) (formula: C₃₄H₅₀N₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			51	34	6	11		
2	B	1	Total	C	N	O	0	0
			51	34	6	11		
2	B	1	Total	C	N	O	0	0
			35	23	4	8		
2	B	1	Total	C	N	O	0	0
			27	19	2	6		
2	C	1	Total	C	N	O	0	0
			51	34	6	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	23	4	8		

- Molecule 3 is GALLIUM (III) ION (three-letter code: GA) (formula: Ga).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ga	0	0
			1	1		
3	B	3	Total	Ga	0	0
			3	3		
3	C	3	Total	Ga	0	0
			3	3		


- Molecule 4 is water.

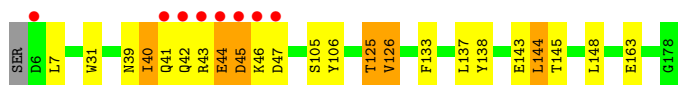
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	76	Total	O	0	0
			76	76		
4	C	47	Total	O	0	0
			47	47		

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: Neutrophil gelatinase-associated lipocalin

Chain A: 




- Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain B: 



- Molecule 1: Neutrophil gelatinase-associated lipocalin

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.34Å 112.17Å 124.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.75 – 2.50 72.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.75-2.50) 100.0 (72.64-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.162 , 0.209 0.169 , 0.217	Depositor DCC
R_{free} test set	1205 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4570	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: F8W, GA

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	0.47	0/1453	0.68	0/1969
1	B	0.46	0/1398	0.68	0/1895
1	C	0.44	0/1390	0.63	0/1884
All	All	0.46	0/4241	0.66	0/5748

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	1415	0	1397	15	0
1	B	1361	0	1348	14	0
1	C	1353	0	1337	5	0
2	A	51	0	0	0	0
2	B	113	0	0	0	0
2	C	86	0	0	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	61	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	76	0	0	2	0
4	C	47	0	0	0	0
All	All	4570	0	4082	34	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 (34) 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:105:SER:HB3	1:A:126:VAL:CG1	2.05	0.86
1:A:125:THR:HG21	4:A:316:HOH:O	1.78	0.83
1:A:105:SER:HB3	1:A:126:VAL:HG13	1.62	0.81
1:B:125:THR:HG21	4:B:315:HOH:O	1.83	0.77
1:B:120:MET:HE2	1:B:155:PHE:CD2	2.23	0.74
1:C:40:ILE:HD12	1:C:41:GLN:C	2.10	0.72
1:A:143:GLU:O	1:A:144:LEU:HD13	2.02	0.59
1:A:42:GLN:HG2	1:A:42:GLN:O	2.03	0.58
1:B:120:MET:CE	1:B:155:PHE:CD2	2.89	0.56
1:B:107:LEU:C	1:B:107:LEU:HD23	2.27	0.55
1:C:40:ILE:HD12	1:C:41:GLN:N	2.22	0.54
1:A:145:THR:HB	4:A:356:HOH:O	2.08	0.52
1:A:137:LEU:HD11	1:A:148:LEU:HD21	1.91	0.52
1:A:144:LEU:HG	1:A:148:LEU:HD22	1.92	0.52
1:B:40:ILE:HG22	1:B:41:GLN:N	2.26	0.50
1:A:43:ARG:O	1:A:44:GLU:HB2	2.12	0.50
1:B:40:ILE:CG2	1:B:41:GLN:N	2.76	0.49
1:B:125:THR:HG22	4:B:344:HOH:O	2.13	0.49
1:A:43:ARG:HG2	1:A:46:LYS:HG3	1.97	0.46
1:A:125:THR:HG22	4:A:332:HOH:O	2.16	0.46
1:A:43:ARG:O	1:A:44:GLU:CB	2.64	0.46
1:B:38:GLU:HB3	1:B:134:TRP:HB3	1.98	0.46
1:C:40:ILE:HD12	1:C:41:GLN:CA	2.47	0.45
1:B:125:THR:HG23	1:B:127:VAL:HG23	1.99	0.45
1:A:40:ILE:CG2	1:A:41:GLN:N	2.80	0.45
1:B:120:MET:HE1	1:B:155:PHE:HB3	1.98	0.44
1:B:144:LEU:O	1:B:149:LYS:HE2	2.19	0.43
1:B:135:ILE:HD11	1:B:159:LEU:HD12	2.00	0.42
1:B:120:MET:CE	1:B:155:PHE:HD2	2.30	0.42
1:B:31:TRP:CE3	1:B:138:TYR:HB3	2.55	0.41
1:A:31:TRP:CE3	1:A:138:TYR:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ASP:HB3	1:C:48:PRO:HD2	2.02	0.40
1:C:31:TRP:CE3	1:C:138:TYR:HB3	2.56	0.40
1:A:39:ASN:HB3	1:A:133:PHE:CE1	2.57	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	171/174 (98%)	163 (95%)	6 (4%)	2 (1%)	13	24
1	B	163/174 (94%)	157 (96%)	6 (4%)	0	100	100
1	C	162/174 (93%)	157 (97%)	5 (3%)	0	100	100
All	All	496/522 (95%)	477 (96%)	17 (3%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	45	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	159/160 (99%)	150 (94%)	9 (6%)	20	39
1	B	153/160 (96%)	146 (95%)	7 (5%)	27	50
1	C	152/160 (95%)	146 (96%)	6 (4%)	32	57
All	All	464/480 (97%)	442 (95%)	22 (5%)	26	49

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	40	ILE
1	A	45	ASP
1	A	47	ASP
1	A	106	TYR
1	A	125	THR
1	A	126	VAL
1	A	144	LEU
1	A	163	GLU
1	B	7	LEU
1	B	15	LYS
1	B	40	ILE
1	B	47	ASP
1	B	98	LYS
1	B	106	TYR
1	B	125	THR
1	C	15	LYS
1	C	47	ASP
1	C	60	GLU
1	C	62	LYS
1	C	106	TYR
1	C	125	THR

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	F8W	B	201	3	52,52,52	1.86	7 (13%)	67,67,67	1.65	10 (14%)
2	F8W	C	203	3	35,35,52	1.26	2 (5%)	45,45,67	1.13	5 (11%)
2	F8W	B	204	3	27,27,52	1.41	2 (7%)	35,35,67	0.87	0
2	F8W	C	201	3	52,52,52	1.47	5 (9%)	67,67,67	1.27	4 (5%)
2	F8W	B	203	3	35,35,52	1.55	4 (11%)	45,45,67	1.37	9 (20%)
2	F8W	A	201	3	52,52,52	1.76	7 (13%)	67,67,67	1.33	7 (10%)

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	F8W	B	201	3	-	10/50/50/50	0/2/2/2
2	F8W	C	203	3	-	10/37/37/50	0/1/1/2
2	F8W	B	204	3	-	1/15/15/50	0/2/2/2
2	F8W	C	201	3	-	8/50/50/50	0/2/2/2
2	F8W	B	203	3	-	9/37/37/50	0/1/1/2
2	F8W	A	201	3	-	6/50/50/50	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	F8W	CAW-CBW	-8.42	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	F8W	CAW-CBW	-7.11	1.46	1.53
2	B	203	F8W	CAC-CAI	-5.53	1.38	1.50
2	A	201	F8W	CAC-CAI	-5.18	1.39	1.50
2	C	201	F8W	CBN-CBM	-5.11	1.39	1.50
2	C	201	F8W	CAW-CBW	-5.09	1.48	1.53
2	C	201	F8W	CAC-CAI	-5.06	1.39	1.50
2	B	201	F8W	CAC-CAI	-4.85	1.40	1.50
2	C	203	F8W	CAC-CAI	-4.82	1.40	1.50
2	B	204	F8W	CAC-CAI	-4.72	1.40	1.50
2	A	201	F8W	CBN-CBM	-4.70	1.40	1.50
2	B	201	F8W	CBN-CBM	-4.62	1.40	1.50
2	A	201	F8W	CAV-CAU	4.58	1.57	1.51
2	B	201	F8W	CAV-CAU	4.38	1.56	1.51
2	B	204	F8W	CBN-CBM	-4.23	1.41	1.50
2	B	203	F8W	CAZ-CBA	3.95	1.56	1.51
2	B	203	F8W	CAW-CBW	3.74	1.57	1.53
2	A	201	F8W	CAZ-CBA	3.61	1.56	1.51
2	C	203	F8W	CAZ-CBA	3.54	1.55	1.51
2	B	203	F8W	CAV-CAU	3.27	1.55	1.51
2	C	201	F8W	CAZ-CBA	2.93	1.55	1.51
2	B	201	F8W	OAY-CAW	2.79	1.48	1.43
2	C	201	F8W	CAV-CAU	2.56	1.54	1.51
2	A	201	F8W	CAV-CAW	2.16	1.56	1.53
2	B	201	F8W	CAZ-CBA	2.16	1.54	1.51
2	A	201	F8W	OAY-CAW	2.10	1.47	1.43
2	B	201	F8W	CAV-CAW	2.07	1.56	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	F8W	OAY-CAW-CBW	-8.51	96.92	108.86
2	C	201	F8W	OBX-CBW-CAW	-6.04	113.70	122.25
2	B	201	F8W	OBX-CBW-CAW	-5.62	114.30	122.25
2	A	201	F8W	OBX-CBW-CAW	-5.22	114.86	122.25
2	A	201	F8W	OAY-CAW-CBW	-4.69	102.28	108.86
2	B	201	F8W	OAY-CAW-CAV	3.36	117.27	109.40
2	B	203	F8W	OBX-CBW-CAW	-3.31	117.57	122.25
2	C	201	F8W	OAY-CAW-CBW	-3.30	104.23	108.86
2	B	201	F8W	OBD-CBA-CAZ	-2.91	118.31	122.14
2	A	201	F8W	CAV-CAW-CBW	-2.82	104.05	110.11
2	C	203	F8W	CAZ-CBA-NBB	2.81	118.46	115.57
2	C	203	F8W	OBX-CBW-CAW	-2.78	118.32	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	F8W	OBD-CBA-CAZ	-2.77	118.50	122.14
2	B	203	F8W	OBY-CBW-CAW	2.74	117.81	113.05
2	C	201	F8W	CBP-CBQ-CBR	-2.74	117.69	120.50
2	B	201	F8W	OBY-CBW-OBX	2.57	131.99	123.82
2	B	203	F8W	OAY-CAW-CAZ	-2.45	103.66	109.40
2	B	203	F8W	CAC-CAD-CAE	-2.44	118.02	120.09
2	A	201	F8W	OAY-CAW-CAV	2.39	114.99	109.40
2	B	201	F8W	CAV-CAU-NAT	2.36	118.00	115.57
2	C	203	F8W	OBD-CBA-CAZ	-2.34	119.07	122.14
2	B	201	F8W	OAY-CAW-CAZ	2.32	114.83	109.40
2	B	203	F8W	CAR-CAS-NAT	-2.24	105.81	112.21
2	C	203	F8W	OBY-CBW-CAW	2.20	116.87	113.05
2	A	201	F8W	OBY-CBW-OBX	2.19	130.80	123.82
2	B	203	F8W	CAM-CAN-NAO	-2.18	106.25	112.14
2	A	201	F8W	CAD-CAE-CAF	2.15	121.76	119.86
2	B	203	F8W	CAM-CAL-NAJ	-2.11	106.17	112.21
2	B	201	F8W	CAD-CAE-CAF	2.11	121.73	119.86
2	B	201	F8W	CAV-CAW-CBW	-2.11	105.58	110.11
2	B	203	F8W	CAZ-CBA-NBB	2.10	117.73	115.57
2	A	201	F8W	CAW-CAV-CAU	2.07	118.87	113.76
2	C	203	F8W	CAR-CAS-NAT	-2.04	106.39	112.21
2	B	201	F8W	CBP-CBQ-CBR	-2.04	118.41	120.50
2	C	201	F8W	OBY-CBW-OBX	2.03	130.26	123.82

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	F8W	CAU-CAV-CAW-OAY
2	C	201	F8W	CAU-CAV-CAW-CAZ
2	A	201	F8W	NBH-CBI-CBJ-CBK
2	C	201	F8W	NBH-CBI-CBJ-CBK
2	B	204	F8W	CBI-CBJ-CBK-NBL
2	B	201	F8W	NBH-CBI-CBJ-CBK
2	A	201	F8W	CAU-CAV-CAW-CAZ
2	B	201	F8W	CAU-CAV-CAW-CAZ
2	C	203	F8W	NBB-CBC-CBE-CBF
2	B	203	F8W	CAB-CAC-CAI-OAK
2	C	203	F8W	CAW-CAZ-CBA-OBD
2	A	201	F8W	CAU-CAV-CAW-OAY
2	B	203	F8W	CAW-CAZ-CBA-NBB
2	C	201	F8W	CAU-CAV-CAW-CBW

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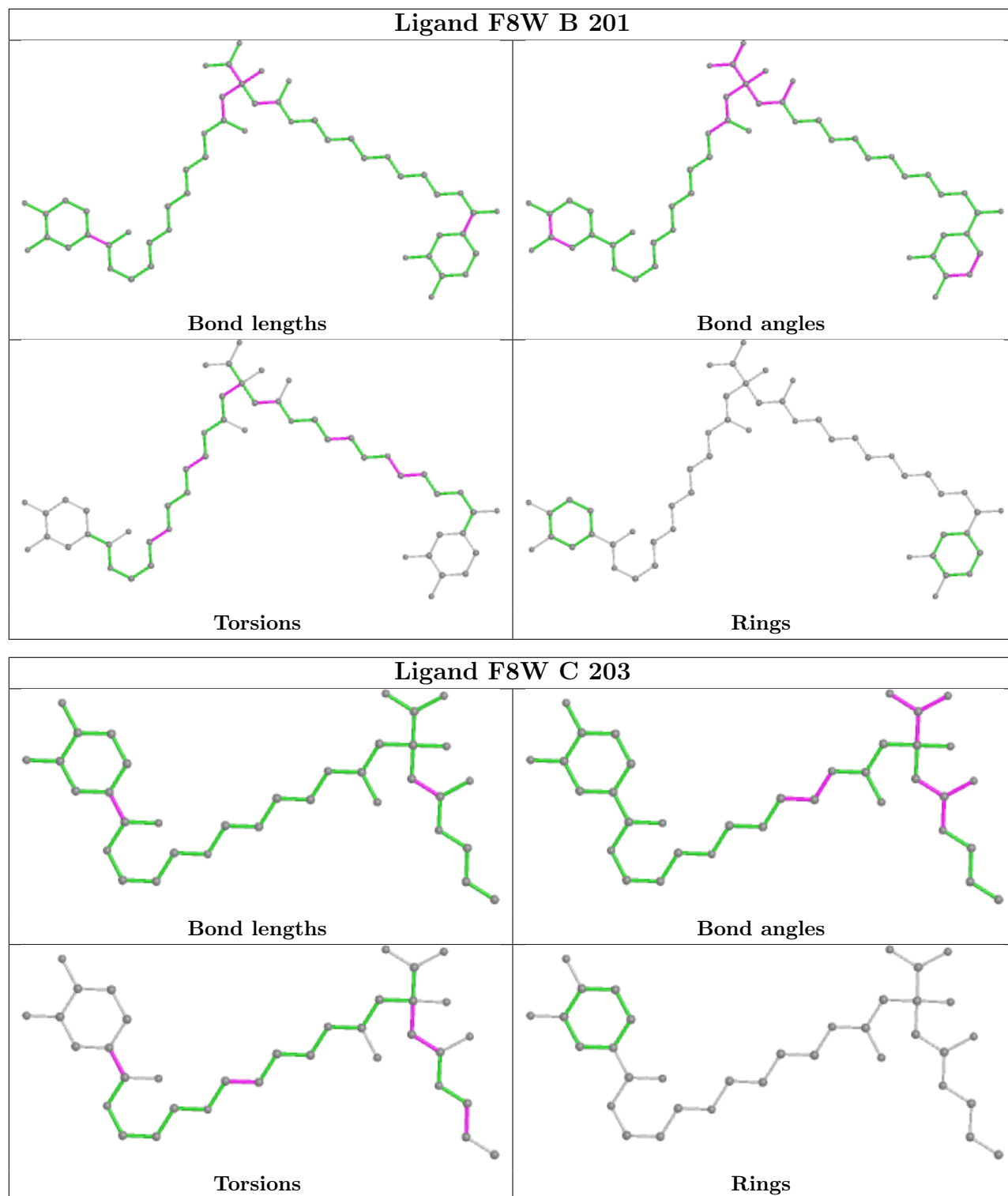
Mol	Chain	Res	Type	Atoms
2	B	203	F8W	CAB-CAC-CAI-NAJ
2	B	203	F8W	CAD-CAC-CAI-OAK
2	C	203	F8W	CAD-CAC-CAI-OAK
2	C	203	F8W	CAB-CAC-CAI-OAK
2	B	203	F8W	CAD-CAC-CAI-NAJ
2	A	201	F8W	CAU-CAV-CAW-CBW
2	C	201	F8W	CAM-CAN-NAO-CAP
2	C	203	F8W	CAW-CAZ-CBA-NBB
2	C	203	F8W	CAD-CAC-CAI-NAJ
2	B	201	F8W	CBC-CBE-CBF-CBG
2	B	203	F8W	CAW-CAZ-CBA-OBD
2	C	203	F8W	CAB-CAC-CAI-NAJ
2	B	203	F8W	NAO-CAP-CAQ-CAR
2	C	201	F8W	CAQ-CAR-CAS-NAT
2	C	203	F8W	OAY-CAW-CAZ-CBA
2	C	201	F8W	CBJ-CBK-NBL-CBM
2	C	203	F8W	CBW-CAW-CAZ-CBA
2	B	201	F8W	CAQ-CAR-CAS-NAT
2	C	203	F8W	NAO-CAP-CAQ-CAR
2	A	201	F8W	CAW-CAZ-CBA-OBD
2	B	201	F8W	CAU-CAV-CAW-OAY
2	B	201	F8W	CAM-CAN-NAO-CAP
2	A	201	F8W	CAW-CAZ-CBA-NBB
2	B	201	F8W	CAW-CAZ-CBA-NBB
2	B	203	F8W	CAQ-CAP-NAO-CAN
2	C	201	F8W	CBJ-CBI-NBH-CBG
2	B	201	F8W	CAW-CAZ-CBA-OBD
2	B	201	F8W	CBJ-CBI-NBH-CBG
2	B	203	F8W	CAL-CAM-CAN-NAO
2	B	201	F8W	CAU-CAV-CAW-CBW

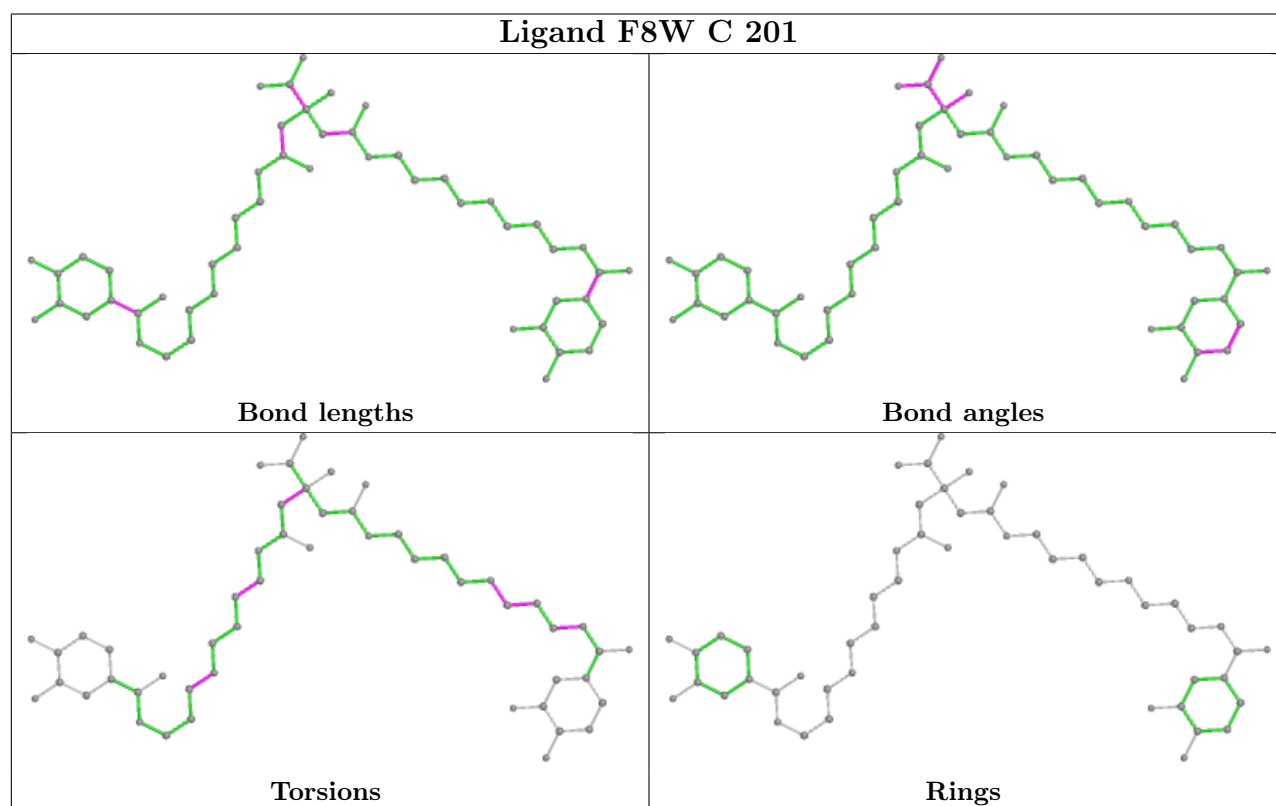
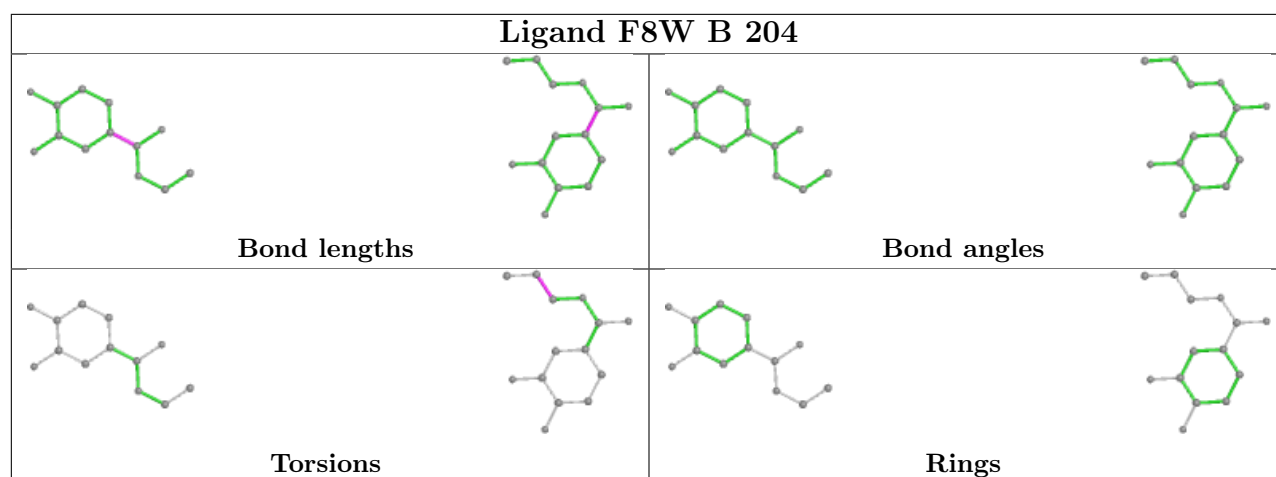
There are no ring outliers.

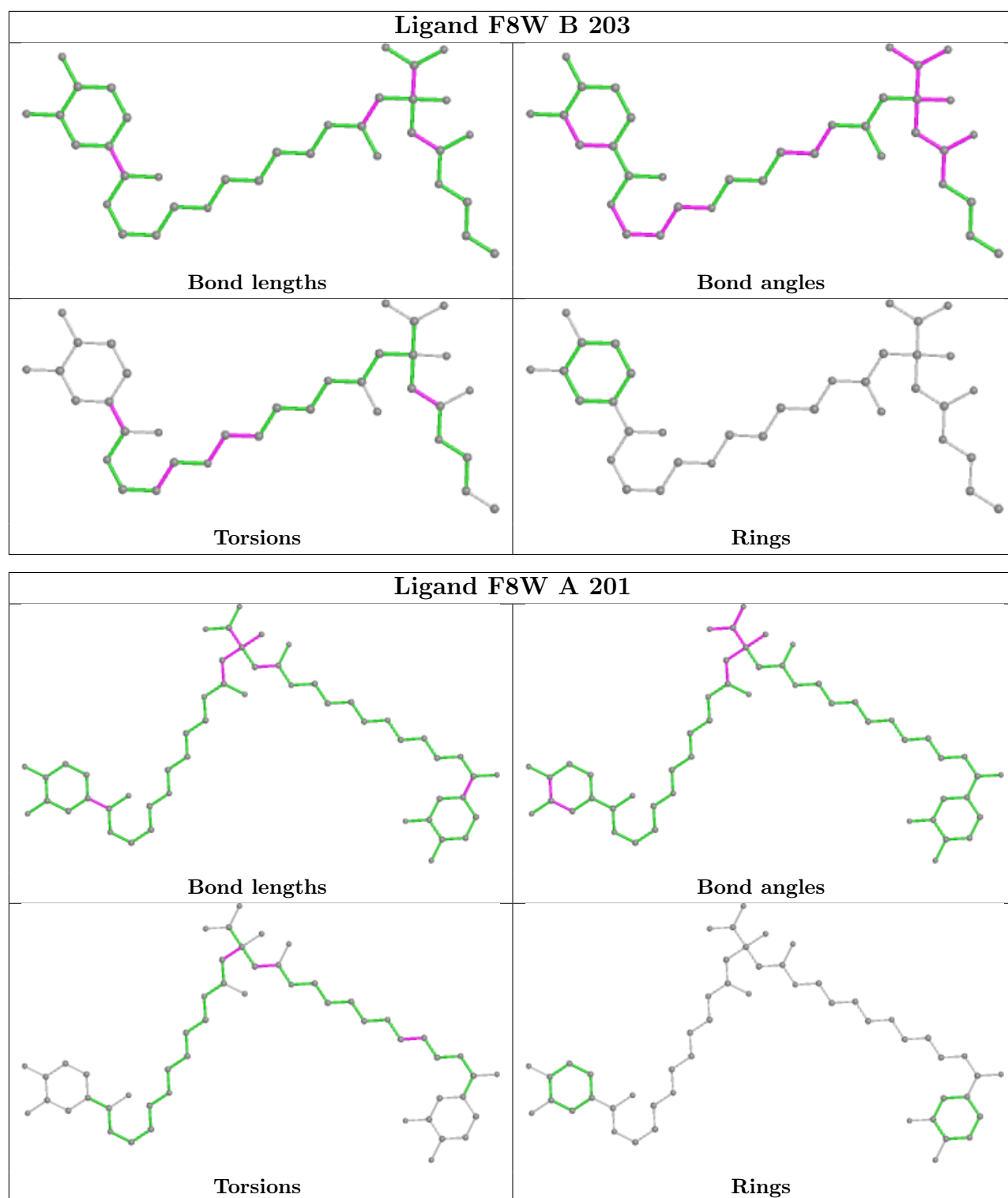
No monomer is involved in short contacts.

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

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	173/174 (99%)	0.20	8 (4%) 32 34	23, 41, 79, 134	0
1	B	167/174 (95%)	-0.09	3 (1%) 68 71	21, 35, 62, 100	0
1	C	166/174 (95%)	0.07	2 (1%) 79 80	22, 43, 71, 100	0
All	All	506/522 (96%)	0.06	13 (2%) 56 59	21, 39, 72, 134	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	GLN	9.7
1	A	44	GLU	8.5
1	A	46	LYS	7.8
1	A	43	ARG	5.9
1	A	45	ASP	5.5
1	B	41	GLN	3.1
1	B	7	LEU	2.7
1	A	41	GLN	2.7
1	C	41	GLN	2.5
1	B	154	ARG	2.5
1	A	47	ASP	2.4
1	A	6	ASP	2.2
1	C	47	ASP	2.2

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](#)

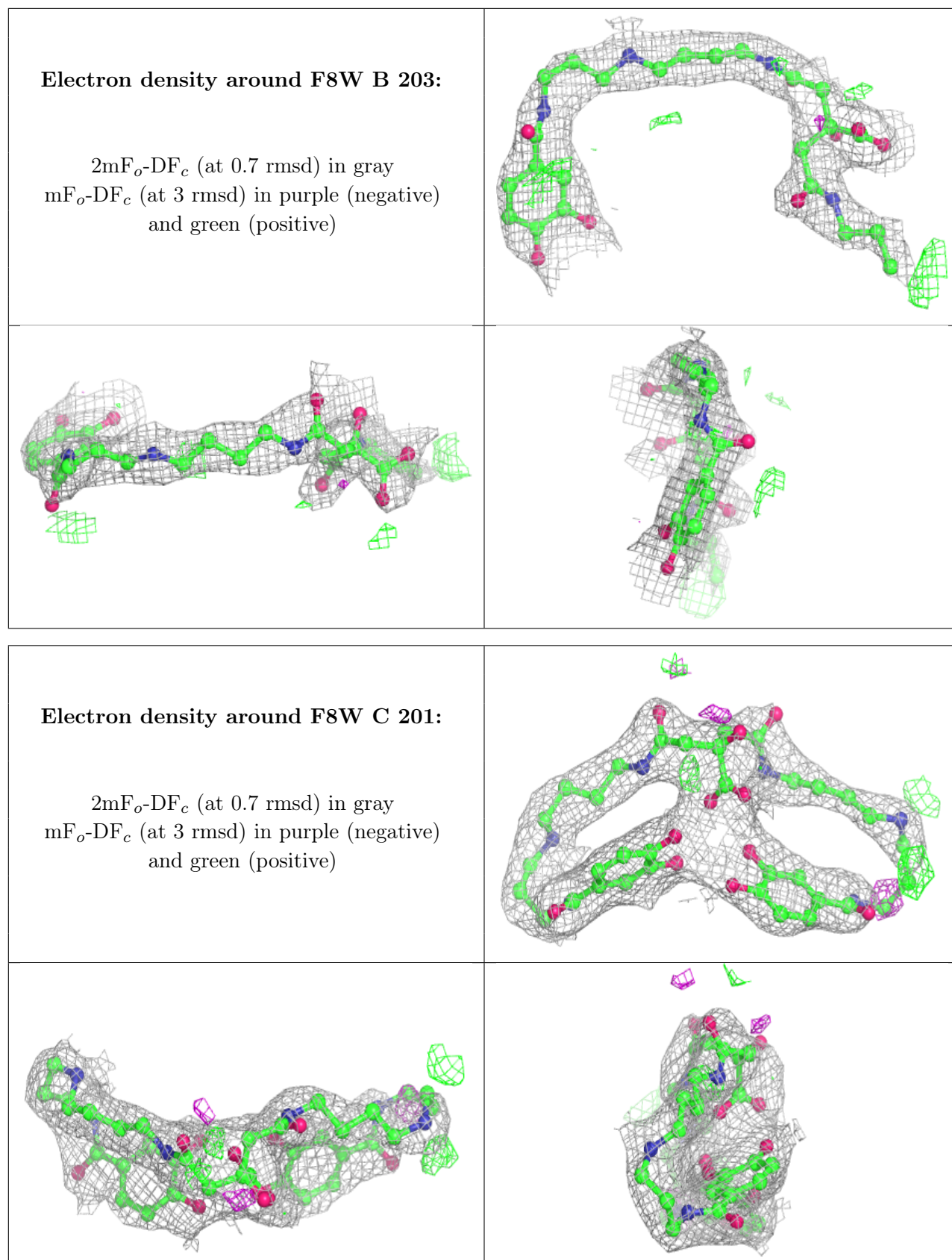
There are no monosaccharides in this entry.

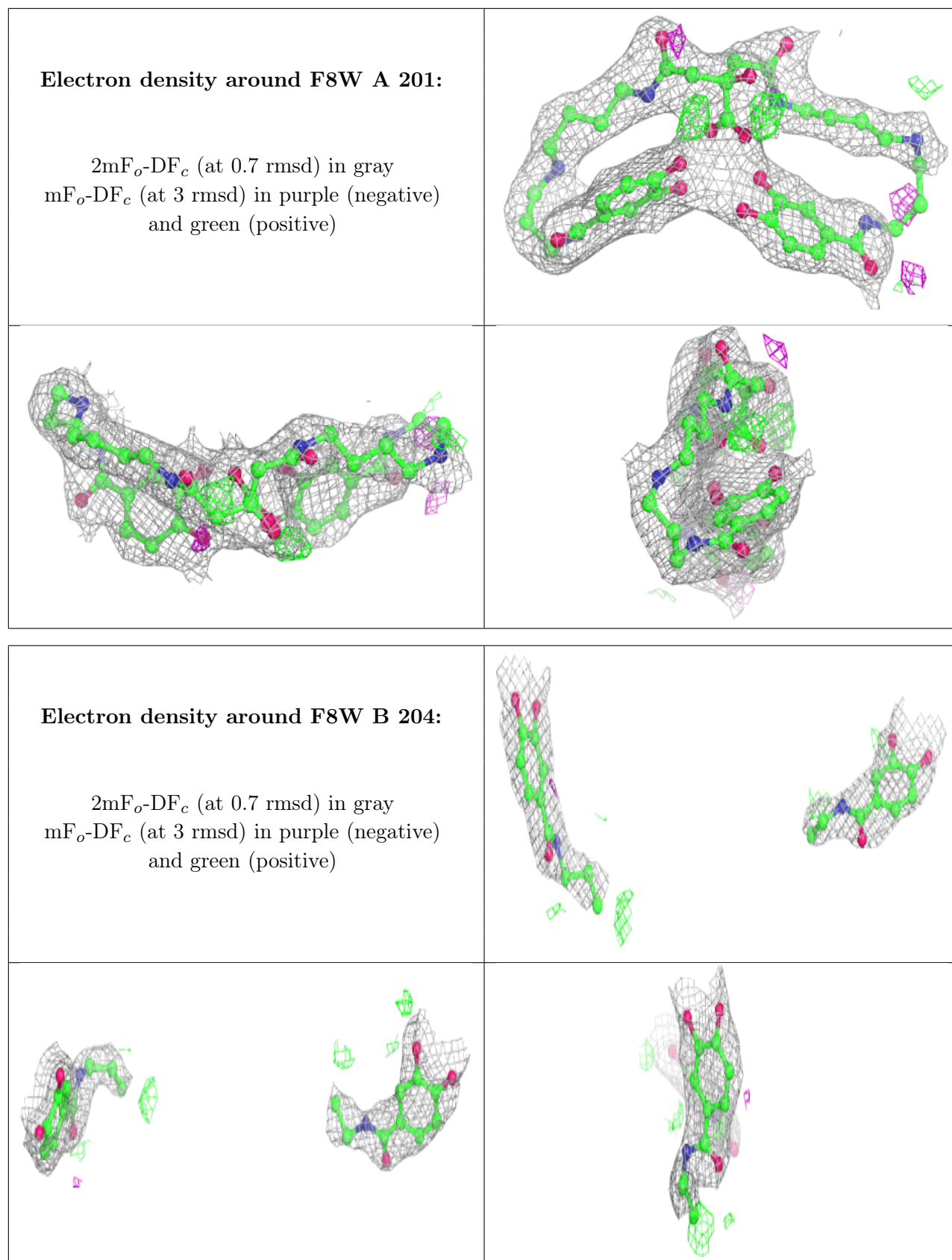
6.4 Ligands

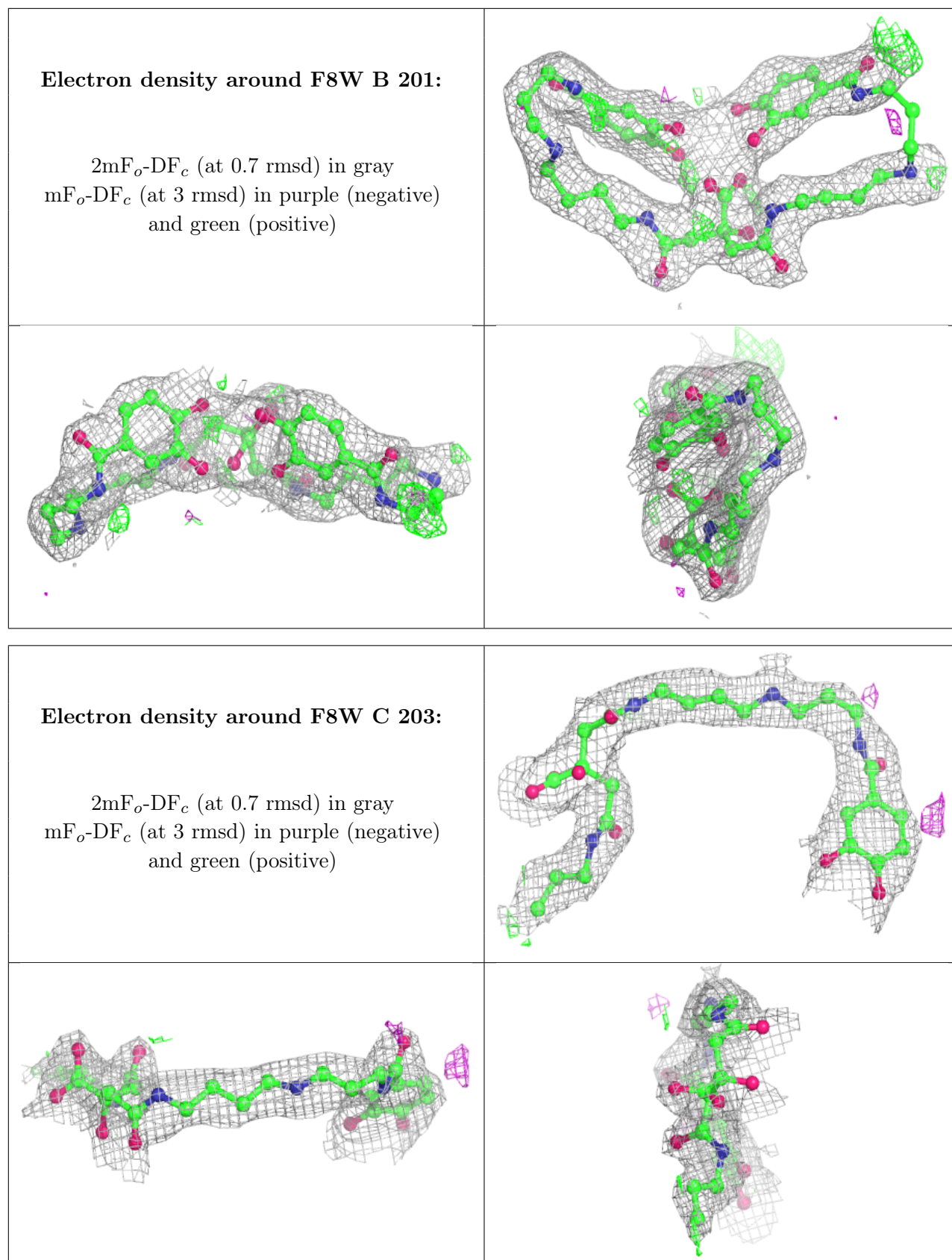
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F8W	B	203	35/51	0.95	0.20	33,41,54,62	0
2	F8W	C	201	51/51	0.96	0.18	30,41,66,79	0
2	F8W	A	201	51/51	0.97	0.16	28,34,67,86	0
2	F8W	B	204	27/51	0.97	0.16	23,46,61,71	0
2	F8W	B	201	51/51	0.97	0.16	20,27,55,66	0
2	F8W	C	203	35/51	0.98	0.16	22,31,39,48	0
3	GA	A	202	1/1	0.99	0.14	34,34,34,34	0
3	GA	C	202	1/1	0.99	0.14	38,38,38,38	0
3	GA	B	205	1/1	1.00	0.11	37,37,37,37	0
3	GA	B	206	1/1	1.00	0.10	33,33,33,33	0
3	GA	B	202	1/1	1.00	0.14	26,26,26,26	0
3	GA	C	204	1/1	1.00	0.16	25,25,25,25	0
3	GA	C	205	1/1	1.00	0.15	25,25,25,25	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.