



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:50 pm BST

PDB ID : 5ZKQ
Title : Crystal structure of the human platelet-activating factor receptor in complex with ABT-491
Authors : Cao, C.; Zhao, Q.; Zhang, X.C.; Wu, B.
Deposited on : 2018-03-25
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

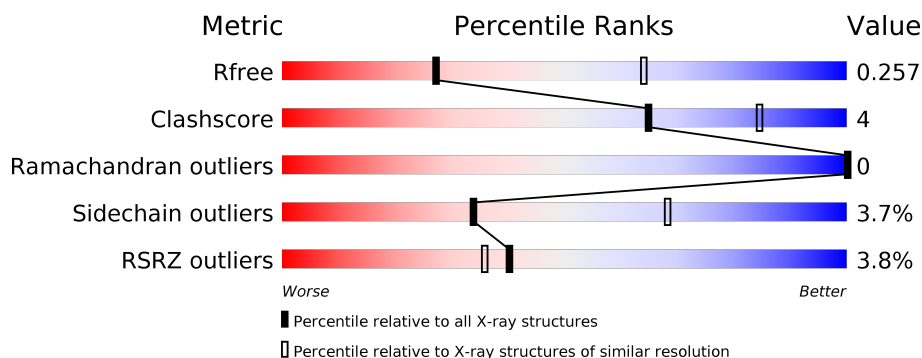
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	438	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>8%</div> <div>36%</div> </div> </div>
1	B	438	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	A	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5568 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 Platelet-activating factor receptor,Endolysin,Endolysin,Platel et-activating factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2178	1452	346	365	15			
1	B	399	Total	C	N	O	S	0	1	0
			3139	2064	523	533	19			

There are 48 discrepancies between the modelled and reference sequences:

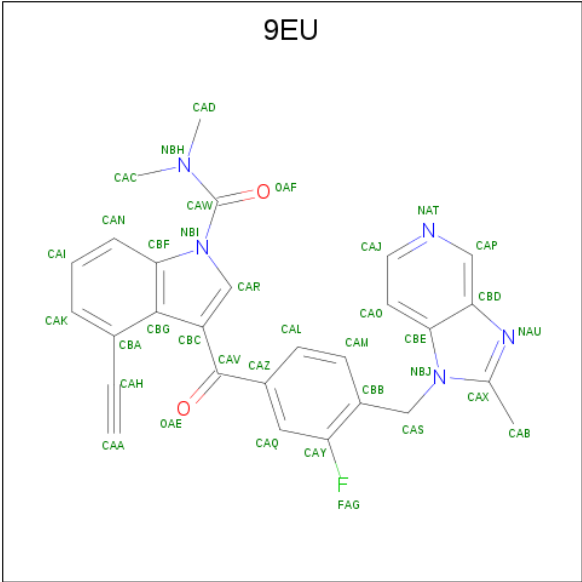
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P25105
A	0	ALA	-	expression tag	UNP P25105
A	1	PRO	-	expression tag	UNP P25105
A	116	TYR	PHE	engineered mutation	UNP P25105
A	169	ASP	ASN	engineered mutation	UNP P25105
A	1011	GLY	-	linker	UNP P00720
A	1012	GLY	-	linker	UNP P00720
A	1013	GLY	-	linker	UNP P00720
A	1014	SER	-	linker	UNP P00720
A	1015	GLY	-	linker	UNP P00720
A	1016	GLY	-	linker	UNP P00720
A	1053	ALA	CYS	engineered mutation	UNP P00720
A	1093	ARG	ILE	engineered mutation	UNP P00720
A	230	ASP	ALA	engineered mutation	UNP P25105
A	234	ALA	VAL	engineered mutation	UNP P25105
A	289	ASN	ASP	engineered mutation	UNP P25105
A	317	GLU	-	expression tag	UNP P25105
A	318	PHE	-	expression tag	UNP P25105
A	319	LEU	-	expression tag	UNP P25105
A	320	GLU	-	expression tag	UNP P25105
A	321	VAL	-	expression tag	UNP P25105
A	322	LEU	-	expression tag	UNP P25105
A	323	PHE	-	expression tag	UNP P25105
A	324	GLN	-	expression tag	UNP P25105

Continued on next page...

Continued from previous page...

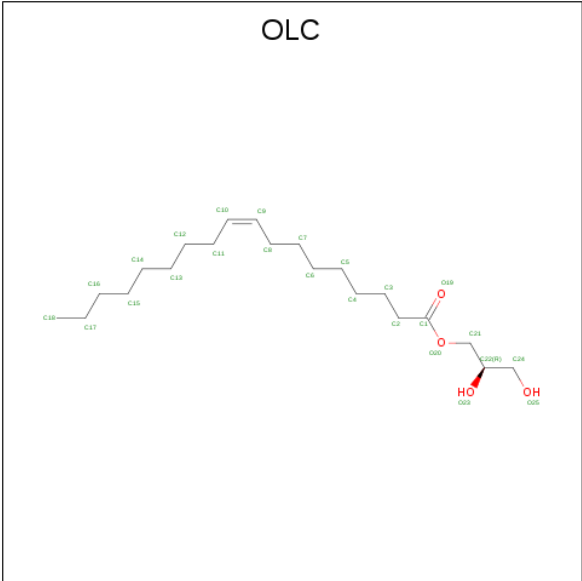
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P25105
B	0	ALA	-	expression tag	UNP P25105
B	1	PRO	-	expression tag	UNP P25105
B	116	TYR	PHE	engineered mutation	UNP P25105
B	169	ASP	ASN	engineered mutation	UNP P25105
B	1011	GLY	-	linker	UNP P00720
B	1012	GLY	-	linker	UNP P00720
B	1013	GLY	-	linker	UNP P00720
B	1014	SER	-	linker	UNP P00720
B	1015	GLY	-	linker	UNP P00720
B	1016	GLY	-	linker	UNP P00720
B	1053	ALA	CYS	engineered mutation	UNP P00720
B	1093	ARG	ILE	engineered mutation	UNP P00720
B	230	ASP	ALA	engineered mutation	UNP P25105
B	234	ALA	VAL	engineered mutation	UNP P25105
B	289	ASN	ASP	engineered mutation	UNP P25105
B	317	GLU	-	expression tag	UNP P25105
B	318	PHE	-	expression tag	UNP P25105
B	319	LEU	-	expression tag	UNP P25105
B	320	GLU	-	expression tag	UNP P25105
B	321	VAL	-	expression tag	UNP P25105
B	322	LEU	-	expression tag	UNP P25105
B	323	PHE	-	expression tag	UNP P25105
B	324	GLN	-	expression tag	UNP P25105

- Molecule 2 is 4-ethynyl-3-{3-fluoro-4-[(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)methyl]benzene-1-carbonyl}-N,N-dimethyl-1H-indole-1-carboxamide (three-letter code: 9EU) (formula: C₂₈H₂₂FN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	B	1	Total	C	F	N	O	0	0
			36	28	1	5	2		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			20	16	4			

Continued on next page...

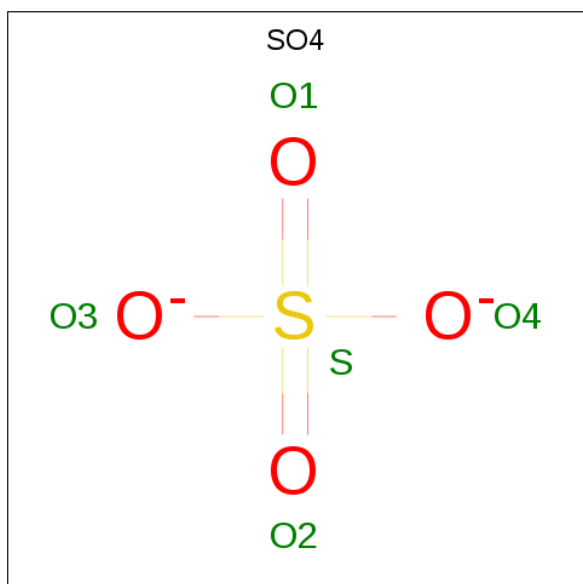
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			12	8	4		
3	B	1	Total	C	O	0	0
			20	16	4		
3	B	1	Total	C	O	0	0
			18	14	4		
3	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

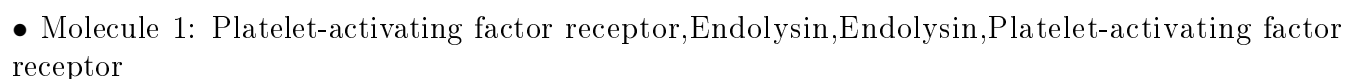
Continued from previous page...

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		

- Molecule 1: Platelet-activating factor receptor,Endolysin,Endolysin,Platelet-activating factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 166.54Å 100.31Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.90 46.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.39-2.90) 99.4 (46.46-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.203 , 0.235 0.218 , 0.257	Depositor DCC
R_{free} test set	1507 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5568	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OLC, 9EU, SO4

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	0.49	0/2238	0.65	0/3065
1	B	0.50	0/3219	0.69	0/4390
All	All	0.50	0/5457	0.67	0/7455

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	2178	0	2132	15	0
1	B	3139	0	3118	25	0
2	A	36	0	0	1	0
2	B	36	0	0	1	0
3	A	82	0	120	3	0
3	B	63	0	90	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	30	0	0	1	0
6	B	2	0	0	0	0
All	All	5568	0	5460	45	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 (45) 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:52:ILE:HG21	1:A:296:LEU:HD13	1.74	0.70
1:A:86:PRO:HD2	1:A:89:LEU:HD12	1.80	0.64
1:B:1043:VAL:HG21	1:B:1074:LEU:HB3	1.82	0.62
1:A:155:LEU:HD23	3:A:503:OLC:H21	1.82	0.61
1:A:112:THR:OG1	1:A:237:VAL:HG11	2.02	0.60
1:B:86:PRO:HD2	1:B:89:LEU:HD12	1.84	0.60
1:A:183:PRO:HB2	3:A:502:OLC:H24	1.86	0.58
1:A:65:LEU:HB3	1:A:96:LEU:HD22	1.87	0.56
1:B:107:PHE:HA	1:B:110:VAL:HG12	1.88	0.55
1:B:1066:GLY:HA2	5:B:1211:SO4:O3	2.07	0.55
1:B:90:CYS:SG	1:B:157:SER:HB2	2.48	0.54
3:B:1202:OLC:H4	3:B:1203:OLC:H4A	1.92	0.50
1:A:74:ILE:O	1:A:78:GLN:HB2	2.12	0.50
1:B:53:LYS:O	1:B:57:VAL:HG23	2.11	0.49
1:A:110:VAL:HG21	1:A:141:ILE:HD11	1.94	0.49
1:B:1070:PHE:O	1:B:1074:LEU:HG	2.13	0.49
2:B:1201:9EU:CAC	2:B:1201:9EU:CAR	2.90	0.49
1:B:226:VAL:HG12	1:B:227:LYS:HG3	1.95	0.49
1:B:66:PHE:HB2	1:B:100:ASN:HB2	1.94	0.48
1:A:65:LEU:O	1:A:68:ILE:HG13	2.13	0.48
1:B:241:PHE:HA	1:B:245:PHE:HD2	1.79	0.47
1:B:297:THR:HG23	1:B:298:LYS:H	1.80	0.47
1:B:136:SER:O	1:B:140:VAL:HG23	2.15	0.47
1:A:232:TRP:HB3	1:A:295:PHE:CE1	2.51	0.46
1:A:90:CYS:SG	1:A:157:SER:HB2	2.55	0.46
3:B:1204:OLC:H4	3:B:1204:OLC:H7A	1.71	0.46
1:B:155:LEU:HD21	3:B:1202:OLC:H4A	1.97	0.46
1:A:246:VAL:O	1:A:250:VAL:HG23	2.16	0.45
1:B:248:HIS:HA	1:B:278:THR:HB	1.99	0.45
1:A:33:ASN:HA	1:A:36:VAL:HG22	2.00	0.43
1:A:289:ASN:O	1:A:292:ILE:HG12	2.18	0.43
1:B:1031:VAL:HA	1:B:1034:ILE:HD12	2.00	0.43
1:B:96:LEU:HD23	1:B:99:ILE:HD12	2.00	0.43
1:B:210:ILE:O	1:B:214:LEU:HB2	2.19	0.43
1:B:44:TYR:H	1:B:45:PRO:HD3	1.83	0.42
2:A:501:9EU:CAC	2:A:501:9EU:CAR	2.98	0.42
1:B:44:TYR:N	1:B:45:PRO:HD3	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:OD1	1:B:172:ARG:HB2	2.20	0.41
1:B:44:TYR:N	1:B:45:PRO:CD	2.83	0.41
1:B:289:ASN:O	1:B:292:ILE:HG12	2.21	0.41
1:B:56:MET:HG2	1:B:292:ILE:CD1	2.51	0.41
1:A:148:ALA:HB1	3:A:502:OLC:H12	2.02	0.41
3:B:1204:OLC:H11A	3:B:1204:OLC:H8A	1.87	0.40
1:B:1058:MET:O	1:B:1062:MET:HG2	2.21	0.40
1:B:242:ILE:O	1:B:247:PRO:HD3	2.20	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	271/438 (62%)	260 (96%)	11 (4%)	0	100	100
1	B	392/438 (90%)	373 (95%)	19 (5%)	0	100	100
All	All	663/876 (76%)	633 (96%)	30 (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	232/384 (60%)	223 (96%)	9 (4%)	32	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	330/384 (86%)	318 (96%)	12 (4%)	35	69
All	All	562/768 (73%)	541 (96%)	21 (4%)	34	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	TRP
1	A	136	SER
1	A	137	LEU
1	A	156	ASP
1	A	204	PHE
1	A	216	GLN
1	A	230	ASP
1	A	272	ASN
1	A	285	ASN
1	B	8	HIS
1	B	37	LEU
1	B	82	ASN
1	B	84	ILE
1	B	121	ARG
1	B	182	VAL
1	B	200	LEU
1	B	214	LEU
1	B	1024	ASN
1	B	1046	SER
1	B	241	PHE
1	B	272	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	B	188	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
5	SO4	B	1207	-	4,4,4	0.20	0	6,6,6	0.35	0
3	OLC	A	504	-	24,24,24	1.22	3 (12%)	25,25,25	0.70	0
5	SO4	B	1208	-	4,4,4	0.19	0	6,6,6	0.24	0
2	9EU	A	501	-	36,40,40	3.40	16 (44%)	38,59,59	1.67	7 (18%)
5	SO4	B	1209	-	4,4,4	0.17	0	6,6,6	0.09	0
3	OLC	B	1204	-	24,24,24	1.05	1 (4%)	25,25,25	0.79	0
5	SO4	B	1211	-	4,4,4	0.22	0	6,6,6	0.35	0
3	OLC	A	502	-	19,19,24	1.13	1 (5%)	20,20,25	0.67	0
3	OLC	A	505	-	11,11,24	0.85	0	12,12,25	0.76	0
5	SO4	B	1206	-	4,4,4	0.11	0	6,6,6	0.20	0
3	OLC	A	503	-	24,24,24	1.15	1 (4%)	25,25,25	0.73	0
3	OLC	B	1202	-	19,19,24	1.10	1 (5%)	20,20,25	0.77	0
5	SO4	B	1210	-	4,4,4	0.23	0	6,6,6	0.27	0
2	9EU	B	1201	-	36,40,40	3.47	18 (50%)	38,59,59	1.71	4 (10%)
3	OLC	B	1203	-	17,17,24	1.15	1 (5%)	18,18,25	0.80	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
3	OLC	A	504	-	-	15/24/24/24	-
2	9EU	A	501	-	-	1/13/22/22	0/5/5/5
3	OLC	B	1204	-	-	12/24/24/24	-
3	OLC	A	502	-	-	10/19/19/24	-
3	OLC	A	505	-	-	8/11/11/24	-
3	OLC	A	503	-	-	15/24/24/24	-
3	OLC	B	1202	-	-	11/19/19/24	-
2	9EU	B	1201	-	-	3/13/22/22	0/5/5/5
3	OLC	B	1203	-	-	8/17/17/24	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	9EU	CBC-CAV	-13.22	1.35	1.50
2	A	501	9EU	CBC-CAV	-12.18	1.36	1.50
2	B	1201	9EU	CAS-CBB	-5.66	1.39	1.51
2	A	501	9EU	CAS-CBB	-5.37	1.40	1.51
2	A	501	9EU	CAR-NBI	-5.17	1.33	1.39
2	B	1201	9EU	CAP-NAT	5.11	1.41	1.32
2	A	501	9EU	CBG-CBF	-5.09	1.36	1.42
2	B	1201	9EU	CAR-NBI	-5.03	1.33	1.39
2	A	501	9EU	CBA-CBG	-5.01	1.36	1.44
2	A	501	9EU	CAP-NAT	4.98	1.41	1.32
2	B	1201	9EU	CBG-CBF	-4.79	1.36	1.42
2	B	1201	9EU	CBA-CBG	-4.64	1.37	1.44
2	B	1201	9EU	CBC-CBG	-4.50	1.35	1.42
3	A	503	OLC	C9-C10	4.33	1.56	1.31
3	A	504	OLC	C9-C10	4.31	1.56	1.31
2	A	501	9EU	CAZ-CAV	-4.26	1.42	1.49
2	A	501	9EU	CBC-CBG	-4.16	1.36	1.42
2	B	1201	9EU	CAZ-CAV	-4.13	1.42	1.49
3	B	1204	OLC	C9-C10	4.09	1.55	1.31
3	A	502	OLC	C9-C10	4.05	1.55	1.31
3	B	1202	OLC	C9-C10	3.82	1.53	1.31
2	A	501	9EU	CAR-CBC	-3.79	1.33	1.38
2	A	501	9EU	CBF-NBI	-3.69	1.34	1.39
2	B	1201	9EU	CAR-CBC	-3.63	1.33	1.38
3	B	1203	OLC	C9-C10	3.55	1.56	1.29
2	A	501	9EU	CBA-CAH	-3.22	1.41	1.44
2	A	501	9EU	CAN-CBF	-3.04	1.35	1.41
2	A	501	9EU	CAO-CBE	-2.91	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	9EU	CAN-CBF	-2.83	1.35	1.41
2	B	1201	9EU	FAG-CAY	-2.79	1.28	1.35
2	B	1201	9EU	CAO-CBE	-2.70	1.35	1.41
2	B	1201	9EU	CAJ-NAT	2.69	1.41	1.33
2	B	1201	9EU	CBF-NBI	-2.67	1.35	1.39
2	B	1201	9EU	CAO-CAJ	2.48	1.39	1.36
2	A	501	9EU	CAJ-NAT	2.38	1.40	1.33
2	A	501	9EU	CAO-CAJ	2.33	1.39	1.36
3	A	504	OLC	O20-C1	2.23	1.39	1.33
2	A	501	9EU	CBE-CBD	-2.22	1.35	1.40
3	A	504	OLC	C2-C1	2.14	1.57	1.50
2	B	1201	9EU	CAQ-CAY	2.12	1.41	1.37
2	B	1201	9EU	OAF-CAW	2.03	1.24	1.22
2	B	1201	9EU	CBE-CBD	-2.01	1.36	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	9EU	CAO-CAJ-NAT	-5.02	117.28	123.81
2	A	501	9EU	CAO-CAJ-NAT	-4.98	117.33	123.81
2	B	1201	9EU	CAK-CBA-CAH	-4.96	115.19	119.95
2	A	501	9EU	CAR-CBC-CAV	-4.45	121.17	127.78
2	A	501	9EU	CAK-CBA-CAH	-4.38	115.74	119.95
2	B	1201	9EU	CAR-CBC-CAV	-4.34	121.32	127.78
2	B	1201	9EU	CAQ-CAY-CBB	-2.59	120.59	123.98
2	A	501	9EU	CAQ-CAY-CBB	-2.44	120.79	123.98
2	A	501	9EU	CAN-CAI-CAK	-2.06	117.71	120.99
2	A	501	9EU	CAS-CBB-CAY	-2.04	118.64	121.23
2	A	501	9EU	CBA-CBG-CBF	-2.01	119.40	122.84

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	OLC	O20-C21-C22-C24
3	A	505	OLC	C21-C22-C24-O25
3	A	505	OLC	O23-C22-C24-O25
3	A	503	OLC	O20-C21-C22-C24
3	B	1202	OLC	C10-C11-C12-C13
3	B	1202	OLC	O20-C21-C22-C24
3	B	1202	OLC	O20-C21-C22-O23
2	B	1201	9EU	NBJ-CAS-CBB-CAY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	503	OLC	O19-C1-O20-C21
3	B	1203	OLC	O19-C1-O20-C21
3	A	503	OLC	C2-C1-O20-C21
3	A	502	OLC	C2-C1-O20-C21
3	B	1203	OLC	C2-C1-O20-C21
3	A	502	OLC	O19-C1-O20-C21
3	A	504	OLC	O20-C21-C22-O23
3	A	503	OLC	O20-C21-C22-O23
3	B	1204	OLC	C4-C5-C6-C7
3	A	504	OLC	O23-C22-C24-O25
3	A	502	OLC	O20-C21-C22-O23
3	A	505	OLC	O20-C21-C22-O23
3	B	1202	OLC	C1-C2-C3-C4
3	A	504	OLC	C2-C1-O20-C21
3	A	502	OLC	O20-C21-C22-C24
3	A	505	OLC	O20-C21-C22-C24
3	A	503	OLC	C13-C14-C15-C16
3	A	504	OLC	C21-C22-C24-O25
3	A	503	OLC	C21-C22-C24-O25
3	B	1202	OLC	C21-C22-C24-O25
3	A	504	OLC	C14-C15-C16-C17
3	B	1204	OLC	C3-C4-C5-C6
3	A	503	OLC	C4-C5-C6-C7
3	A	503	OLC	C2-C3-C4-C5
3	B	1202	OLC	C5-C6-C7-C8
3	A	503	OLC	C5-C6-C7-C8
3	B	1203	OLC	C2-C3-C4-C5
3	A	503	OLC	C3-C4-C5-C6
3	A	504	OLC	O19-C1-O20-C21
3	B	1202	OLC	O19-C1-O20-C21
3	B	1204	OLC	C6-C7-C8-C9
3	A	503	OLC	C12-C13-C14-C15
3	B	1204	OLC	C14-C15-C16-C17
3	B	1204	OLC	O19-C1-O20-C21
3	B	1204	OLC	C2-C1-O20-C21
3	B	1202	OLC	C2-C1-O20-C21
3	B	1202	OLC	C2-C3-C4-C5
3	A	504	OLC	C3-C4-C5-C6
3	A	504	OLC	C10-C11-C12-C13
3	A	503	OLC	C10-C11-C12-C13
3	B	1204	OLC	C10-C11-C12-C13
3	A	504	OLC	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	505	OLC	C2-C1-O20-C21
3	A	504	OLC	C2-C3-C4-C5
3	A	504	OLC	C1-C2-C3-C4
3	A	502	OLC	C10-C11-C12-C13
3	B	1204	OLC	C2-C3-C4-C5
3	B	1204	OLC	C5-C6-C7-C8
3	B	1203	OLC	C6-C7-C8-C9
3	A	505	OLC	O19-C1-O20-C21
3	A	502	OLC	C3-C4-C5-C6
3	A	505	OLC	C2-C3-C4-C5
3	B	1203	OLC	C5-C6-C7-C8
3	A	503	OLC	C14-C15-C16-C17
3	A	502	OLC	C5-C6-C7-C8
3	B	1202	OLC	O23-C22-C24-O25
3	A	502	OLC	C6-C7-C8-C9
3	B	1203	OLC	C3-C4-C5-C6
3	A	504	OLC	O20-C1-C2-C3
2	A	501	9EU	NBJ-CAS-CBB-CAY
3	A	503	OLC	C9-C10-C11-C12
3	B	1204	OLC	C15-C16-C17-C18
3	A	504	OLC	C12-C13-C14-C15
3	A	504	OLC	C13-C14-C15-C16
3	B	1203	OLC	C21-C22-C24-O25
2	B	1201	9EU	NBI-CAW-NBH-CAC
3	B	1202	OLC	C7-C8-C9-C10
3	B	1203	OLC	O23-C22-C24-O25
3	A	502	OLC	C9-C10-C11-C12
2	B	1201	9EU	NBJ-CAS-CBB-CAM
3	A	502	OLC	O20-C1-C2-C3
3	B	1204	OLC	O20-C1-C2-C3
3	A	503	OLC	O23-C22-C24-O25
3	A	505	OLC	O20-C1-C2-C3
3	B	1204	OLC	C1-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 10 short contacts:

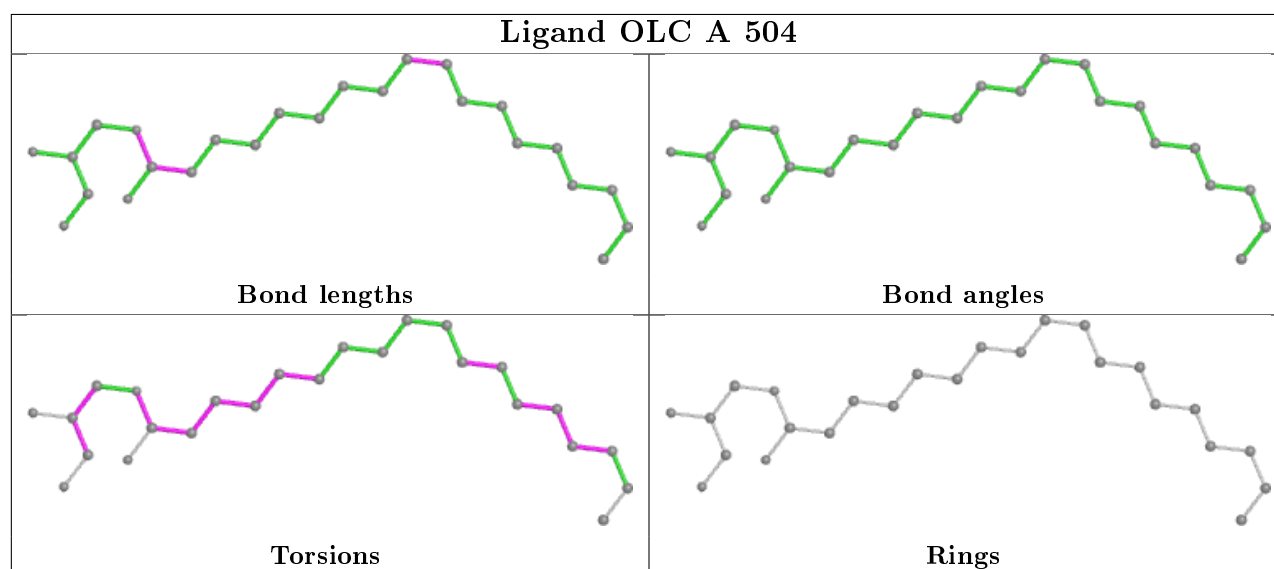
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	9EU	1	0
3	B	1204	OLC	2	0
5	B	1211	SO4	1	0
3	A	502	OLC	2	0

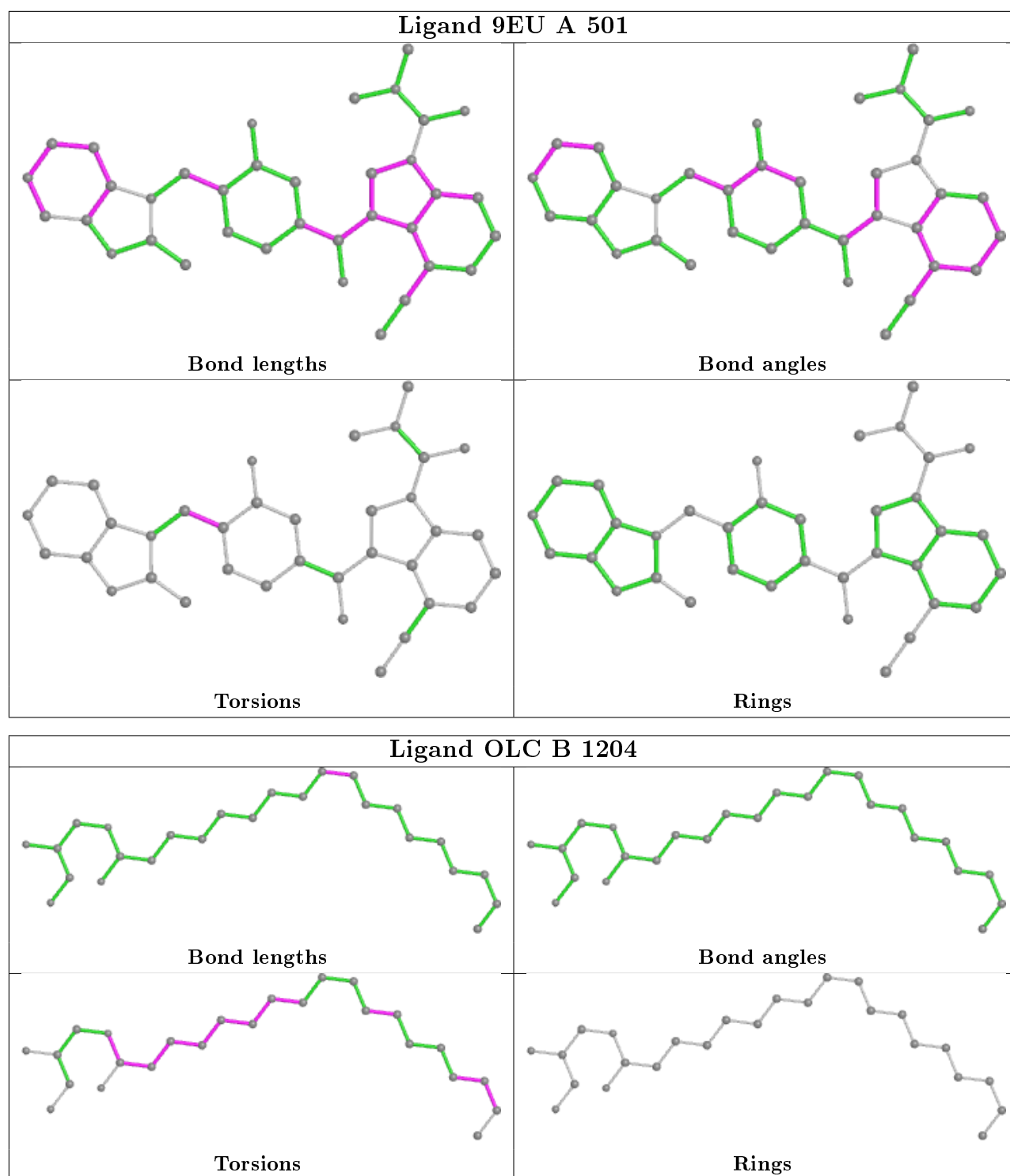
Continued on next page...

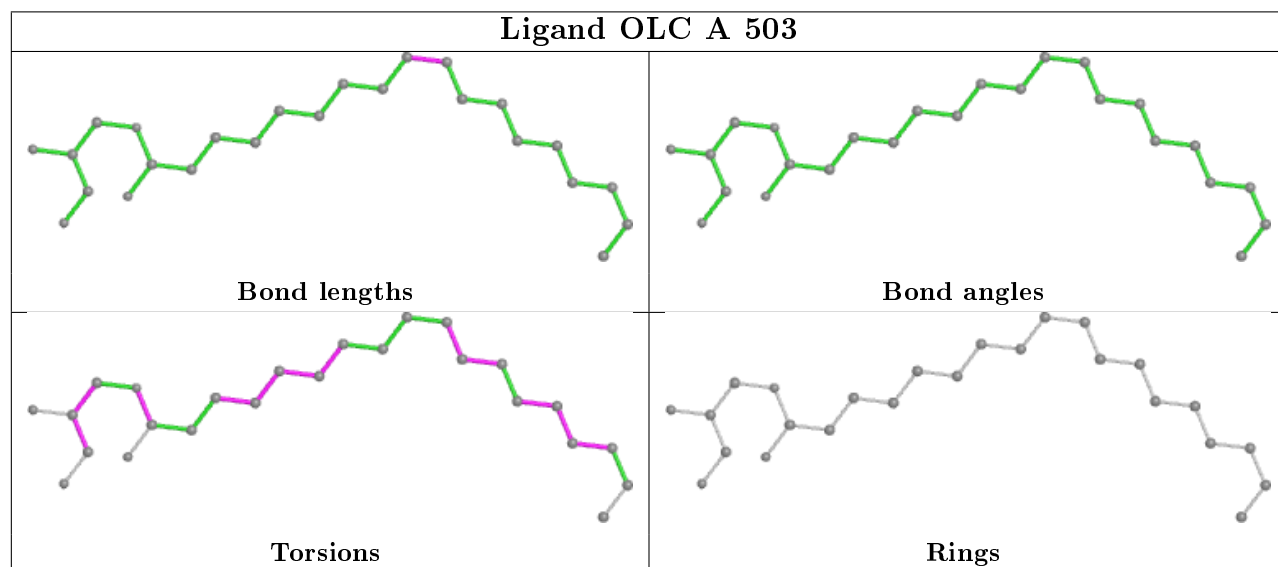
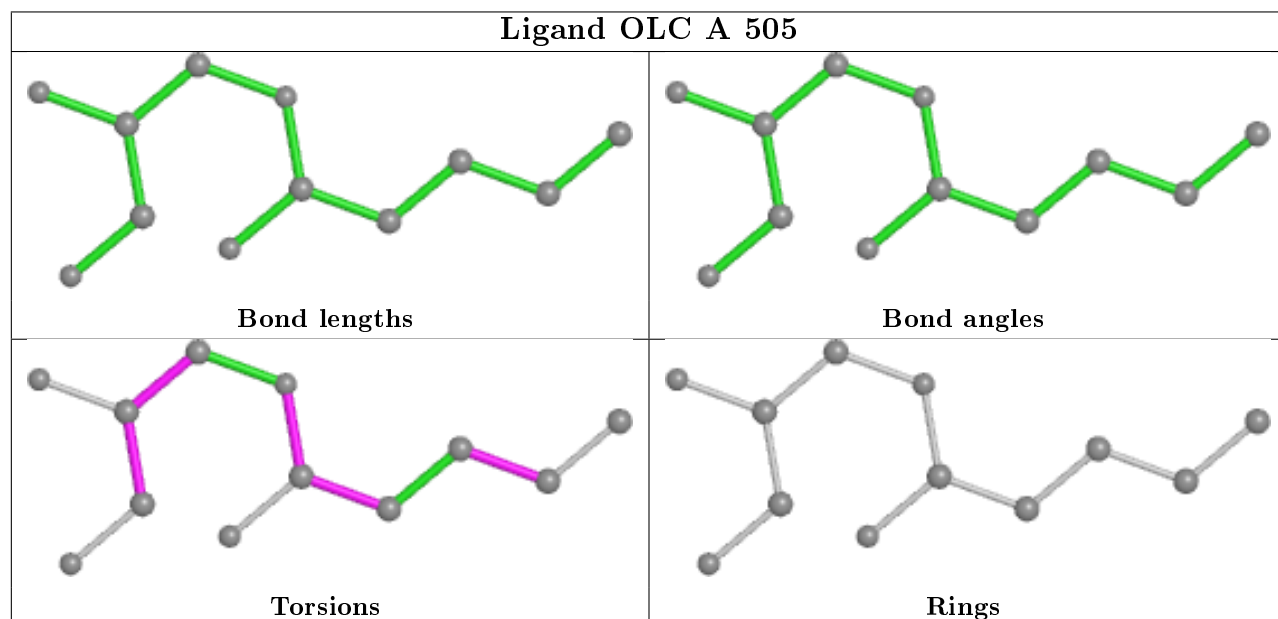
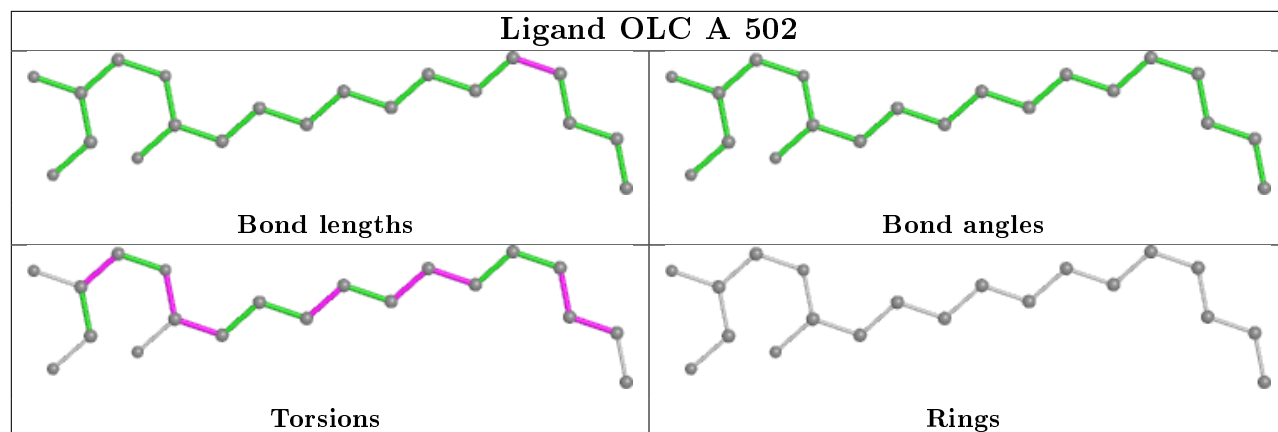
Continued from previous page...

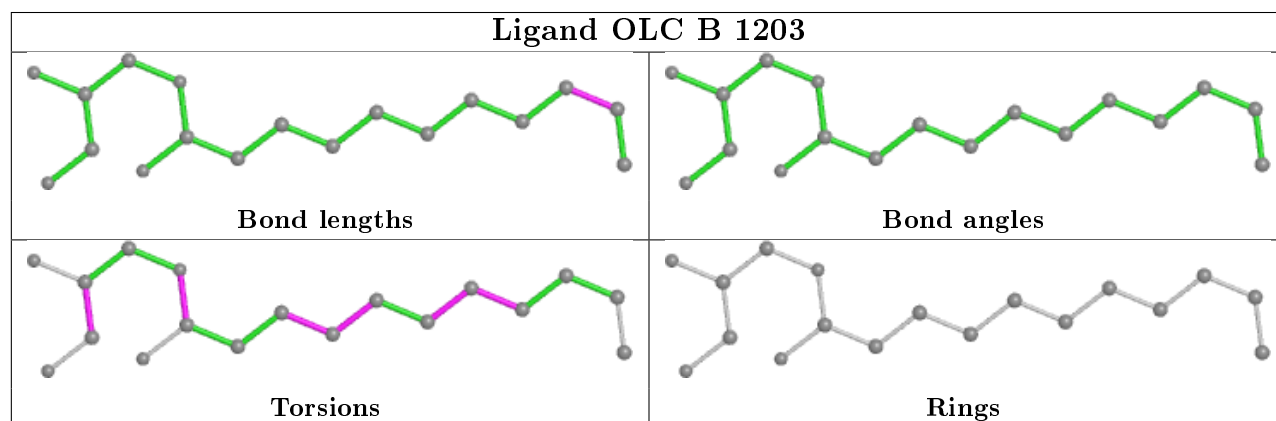
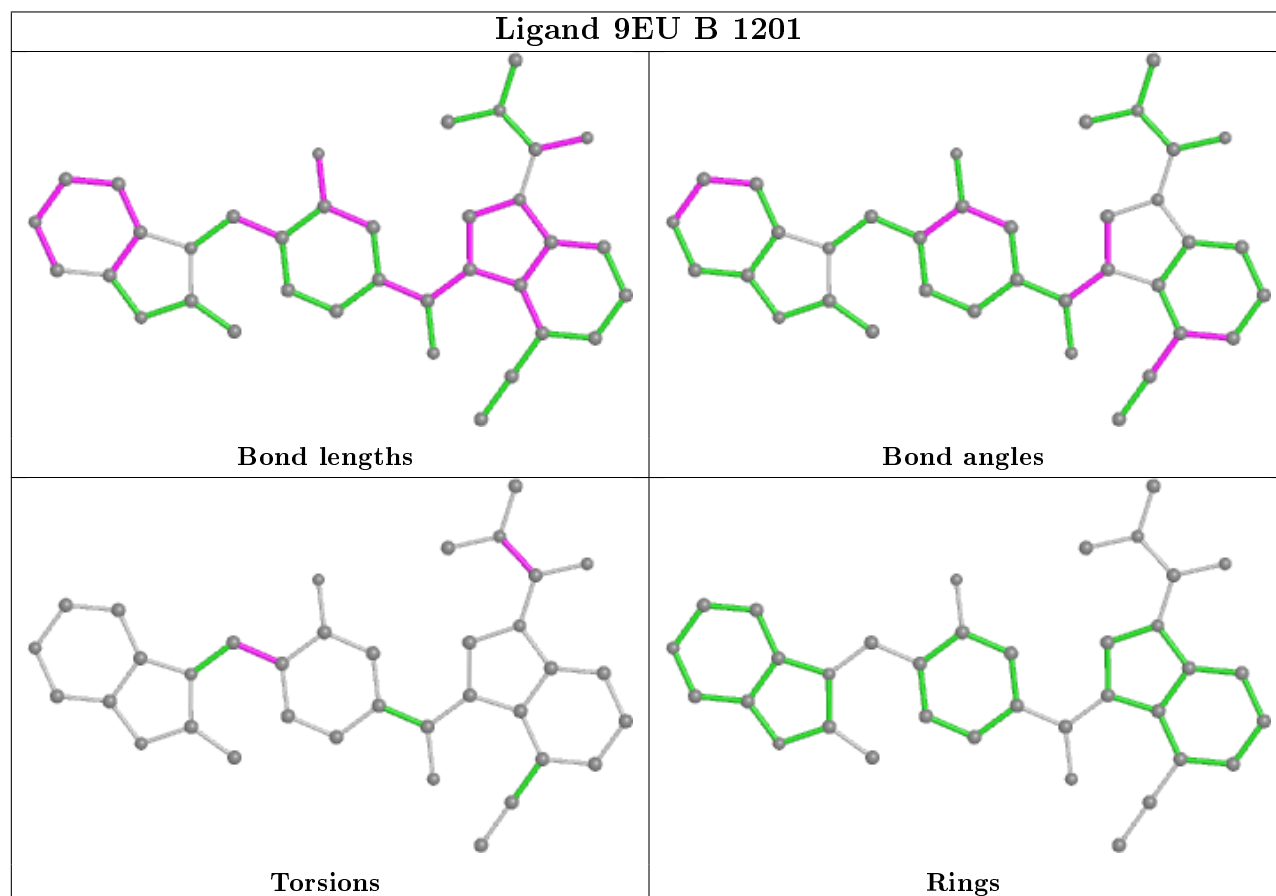
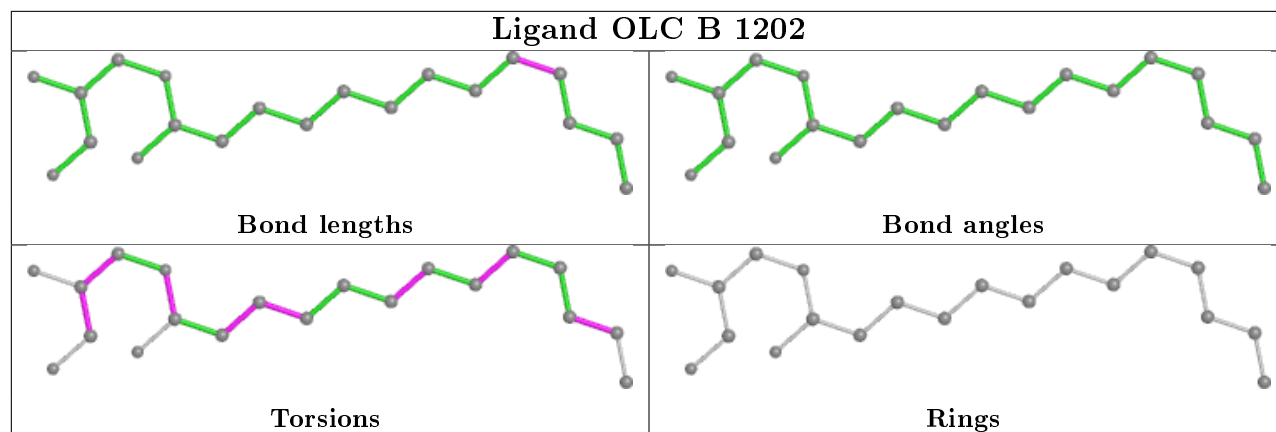
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	OLC	1	0
3	B	1202	OLC	2	0
2	B	1201	9EU	1	0
3	B	1203	OLC	1	0

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 ⓘ

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, 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	279/438 (63%)	0.26	17 (6%) 21 17	60, 89, 143, 159	0
1	B	399/438 (91%)	0.00	9 (2%) 60 58	54, 73, 127, 155	0
All	All	678/876 (77%)	0.11	26 (3%) 40 36	54, 79, 139, 159	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	GLN	6.6
1	B	127	GLN	6.3
1	A	118	ALA	5.0
1	A	128	ALA	4.6
1	A	212	THR	4.5
1	B	45	PRO	4.5
1	A	226	VAL	4.3
1	A	122	PRO	3.7
1	A	167	SER	3.6
1	A	129	ASN	3.5
1	A	213	LEU	3.2
1	A	224	ALA	3.2
1	B	1017	ASP	3.1
1	B	44	TYR	3.0
1	B	1015	GLY	3.0
1	B	265	SER	2.8
1	A	49	PHE	2.8
1	B	128	ALA	2.8
1	A	130	THR	2.6
1	A	215	MET	2.6
1	A	217	PRO	2.6
1	A	10	ASP	2.4
1	B	11	SER	2.2
1	A	119	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	42	ARG	2.1
1	A	211	ARG	2.1

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 carbohydrates in this entry.

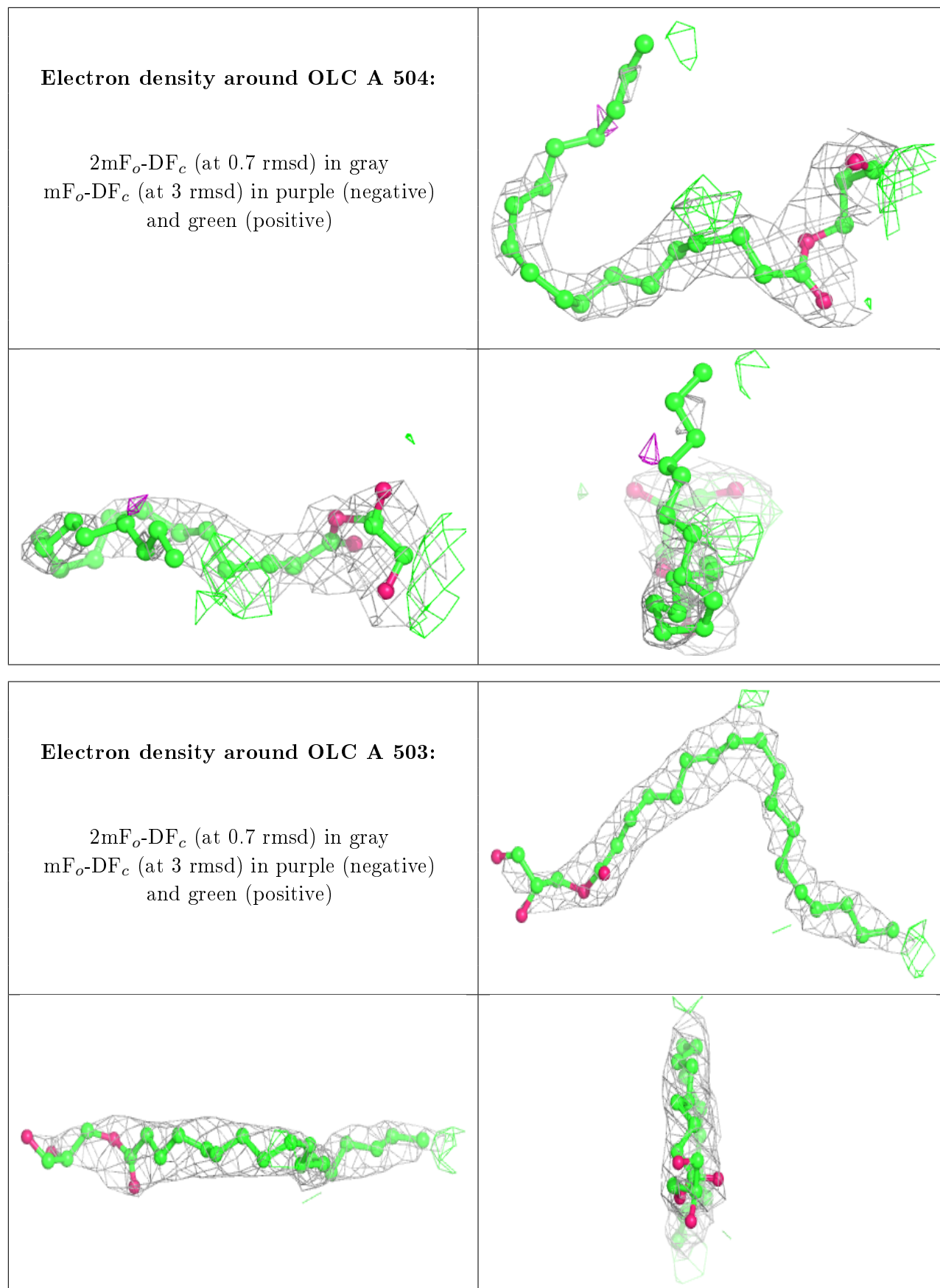
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	OLC	A	504	25/25	0.71	0.41	85,96,107,108	0
3	OLC	A	503	25/25	0.75	0.32	69,81,112,112	0
3	OLC	B	1203	18/25	0.75	0.29	88,97,108,109	0
3	OLC	A	505	12/25	0.79	0.31	98,102,103,105	0
3	OLC	B	1202	20/25	0.83	0.26	76,97,128,129	0
3	OLC	A	502	20/25	0.83	0.28	75,92,117,117	0
3	OLC	B	1204	25/25	0.84	0.40	88,97,104,105	0
5	SO4	B	1209	5/5	0.86	0.17	172,172,173,173	0
5	SO4	B	1206	5/5	0.90	0.23	149,149,149,150	0
4	ZN	B	1205	1/1	0.94	0.08	142,142,142,142	0
5	SO4	B	1211	5/5	0.95	0.13	101,103,104,105	0
2	9EU	B	1201	36/36	0.97	0.16	65,84,92,93	0
5	SO4	B	1210	5/5	0.98	0.12	90,90,91,92	0
5	SO4	B	1208	5/5	0.98	0.17	76,80,81,84	0
2	9EU	A	501	36/36	0.98	0.20	76,82,87,93	0
5	SO4	B	1207	5/5	0.99	0.14	77,80,82,83	0
4	ZN	A	506	1/1	0.99	0.09	121,121,121,121	0

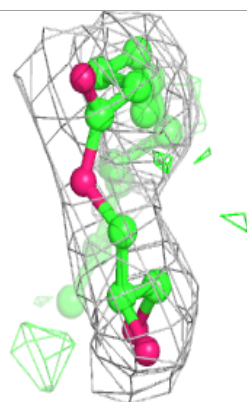
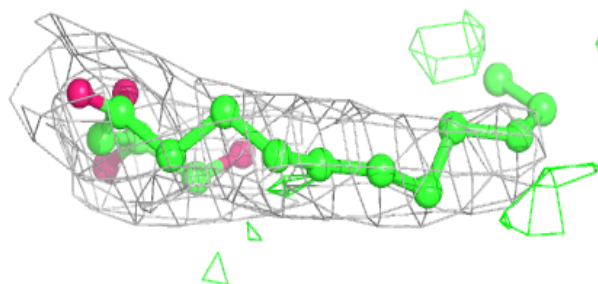
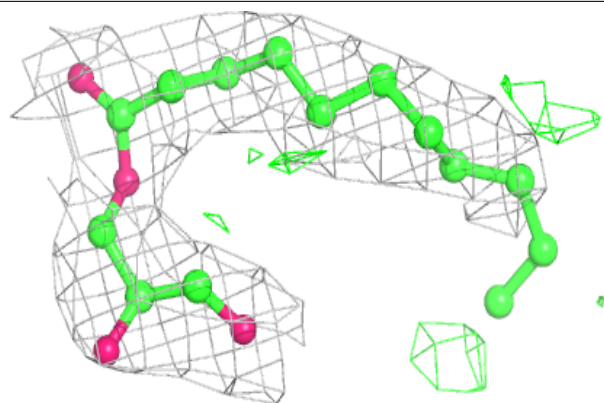
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

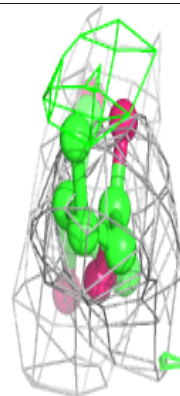
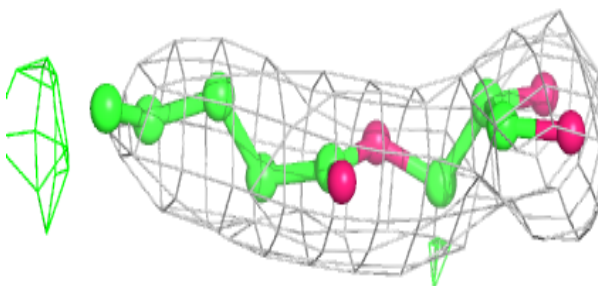
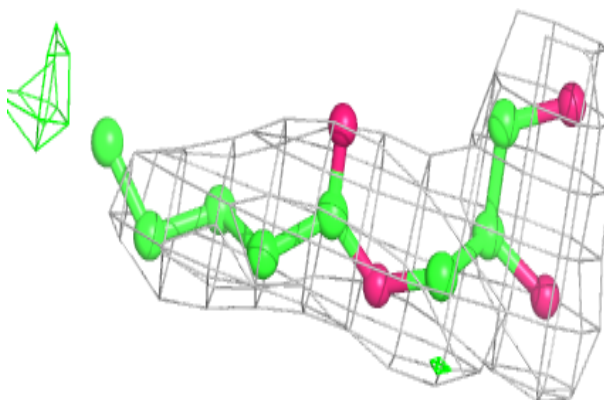


Electron density around OLC B 1203:

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

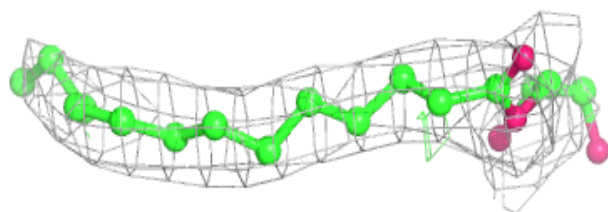
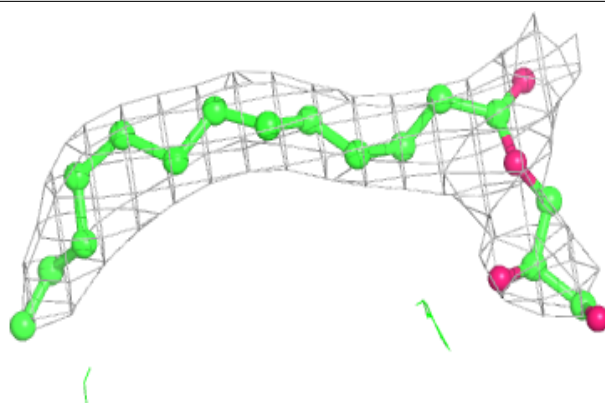
**Electron density around OLC A 505:**

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

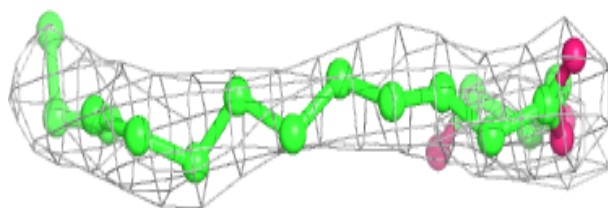
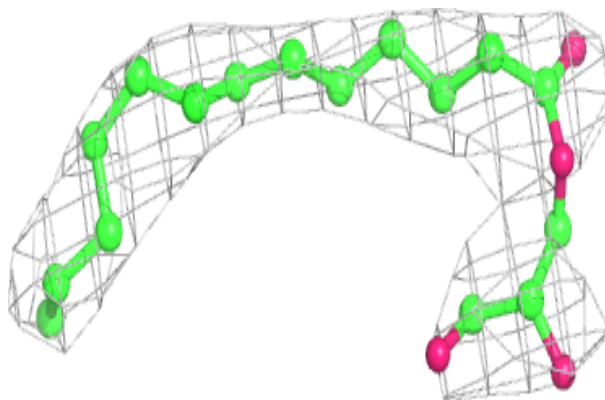


Electron density around OLC B 1202:

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

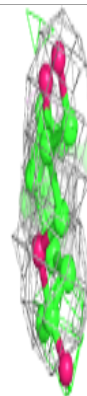
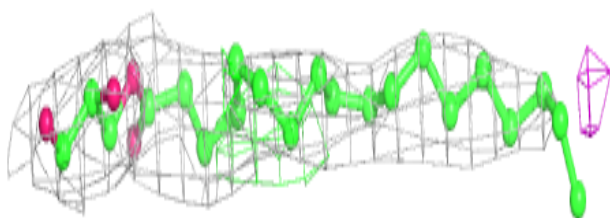
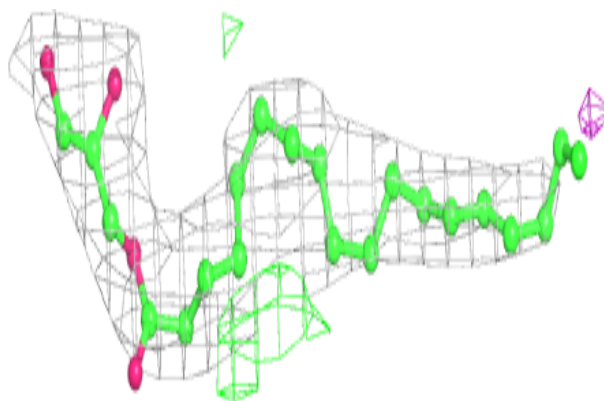
**Electron density around OLC A 502:**

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

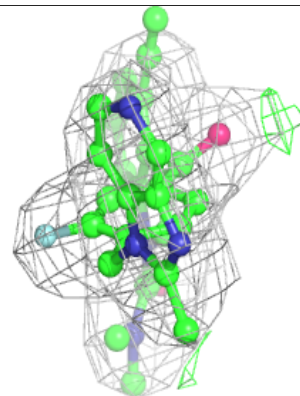
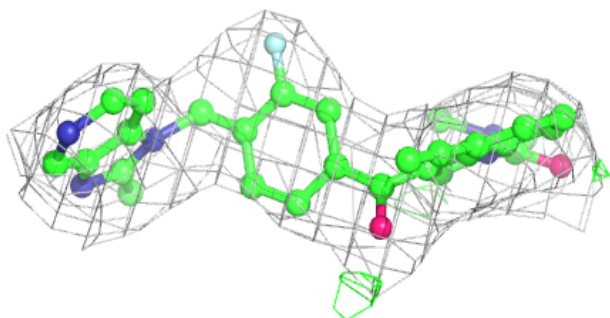
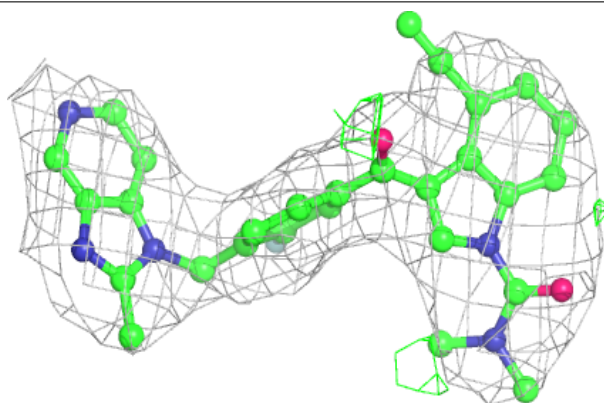


Electron density around OLC B 1204:

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

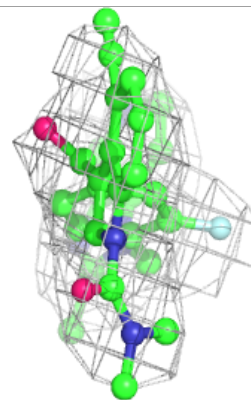
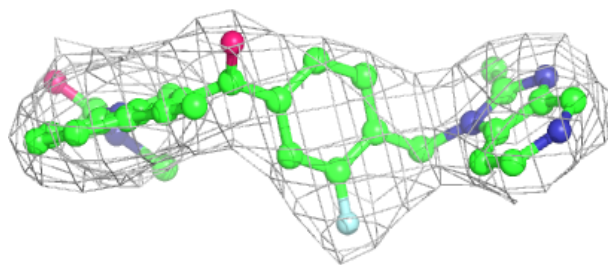
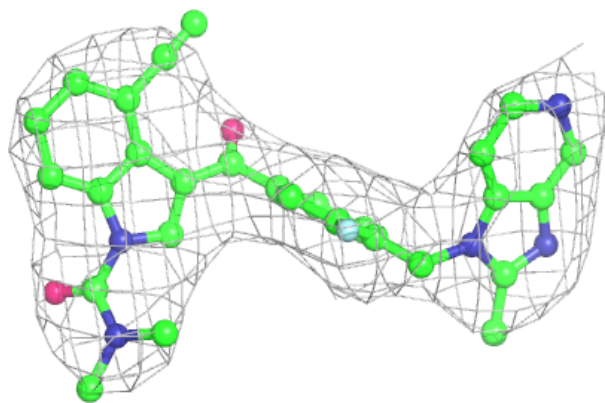
**Electron density around 9EU B 1201:**

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



Electron density around 9EU A 501:

$2mF_o-DF_c$ (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.