



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:00 am BST

PDB ID : 6C1R
Title : Crystal structure of human C5a receptor in complex with an orthosteric antagonist PMX53 and an allosteric antagonist avacopan
Authors : Liu, H.; Wang, L.; Wei, Z.; Zhang, C.
Deposited on : 2018-01-05
Resolution : 2.20 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

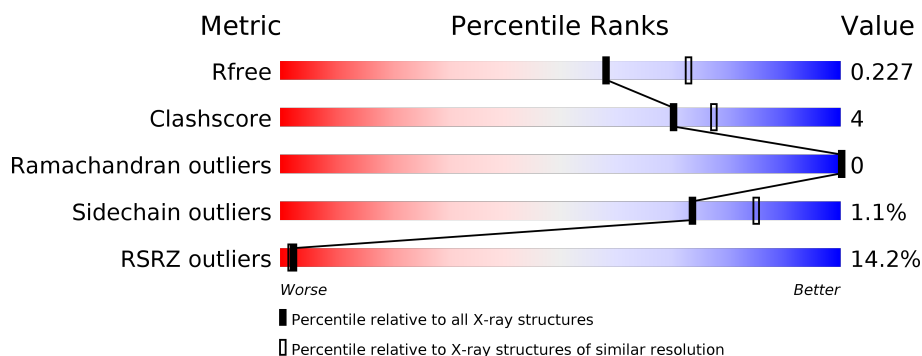
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	B	422	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>12%</div> </div> </div>
2	L	7	<div> <div>86%</div> <div>14%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3087 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 Soluble cytochrome b562, C5a anaphylatoxin chemotactic receptor 1 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	371	Total	C	N	O	S	0	0	0
			2781	1839	456	473	13			

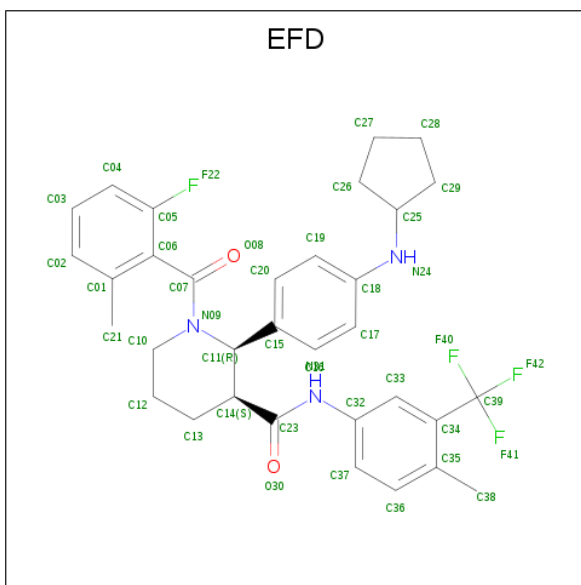
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ASP	-	expression tag	UNP P0ABE7
B	2	TYR	-	expression tag	UNP P0ABE7
B	3	LYS	-	expression tag	UNP P0ABE7
B	4	ASP	-	expression tag	UNP P0ABE7
B	5	ASP	-	expression tag	UNP P0ABE7
B	6	ASP	-	expression tag	UNP P0ABE7
B	7	ASP	-	expression tag	UNP P0ABE7
B	8	VAL	-	expression tag	UNP P0ABE7
B	9	ASP	-	expression tag	UNP P0ABE7
B	16	TRP	MET	engineered mutation	UNP P0ABE7
B	111	ILE	HIS	engineered mutation	UNP P0ABE7
B	115	LEU	ARG	engineered mutation	UNP P0ABE7
B	418	ASN	-	expression tag	UNP P21730
B	419	LEU	-	expression tag	UNP P21730
B	420	TYR	-	expression tag	UNP P21730
B	421	PHE	-	expression tag	UNP P21730
B	422	GLN	-	expression tag	UNP P21730

- Molecule 2 is a protein called PMX53.

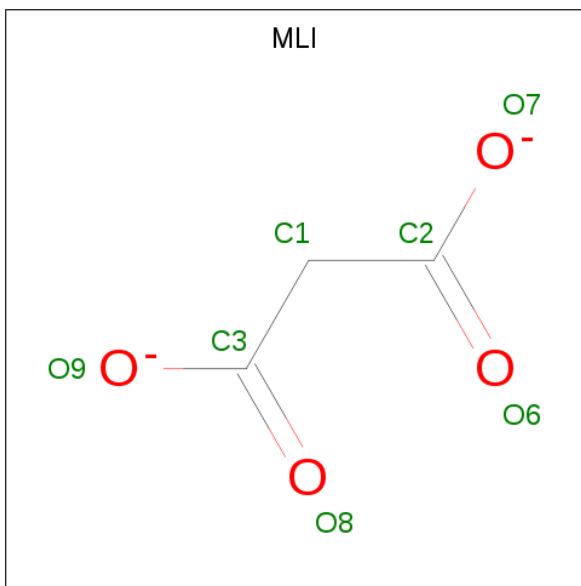
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	7	Total	C	N	O	0	0	0
			65	47	11	7			

- Molecule 3 is avacopan (three-letter code: EFD) (formula: C₃₃H₃₅F₄N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			42	33	4	3	2		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).

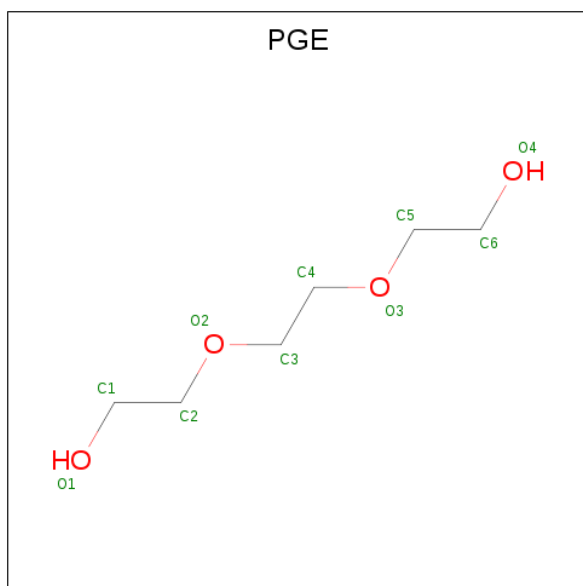


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

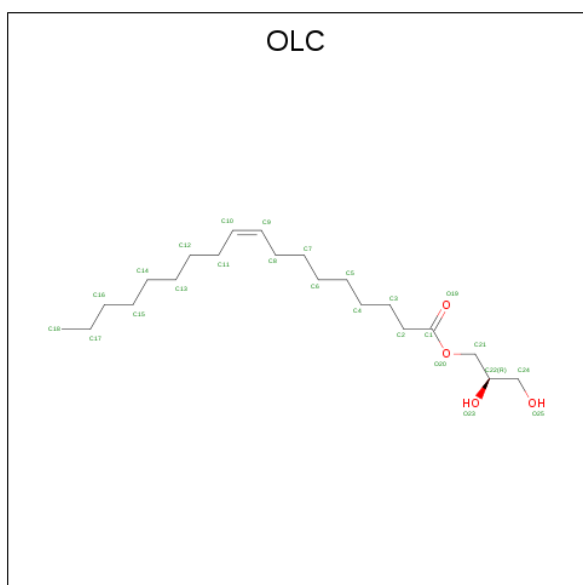
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



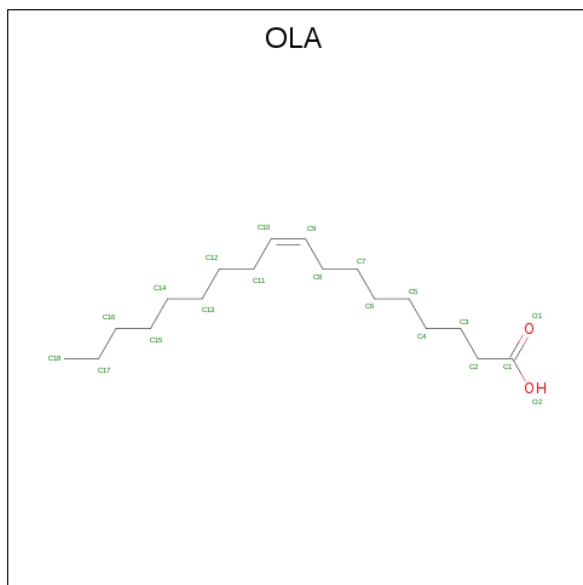
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 8 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

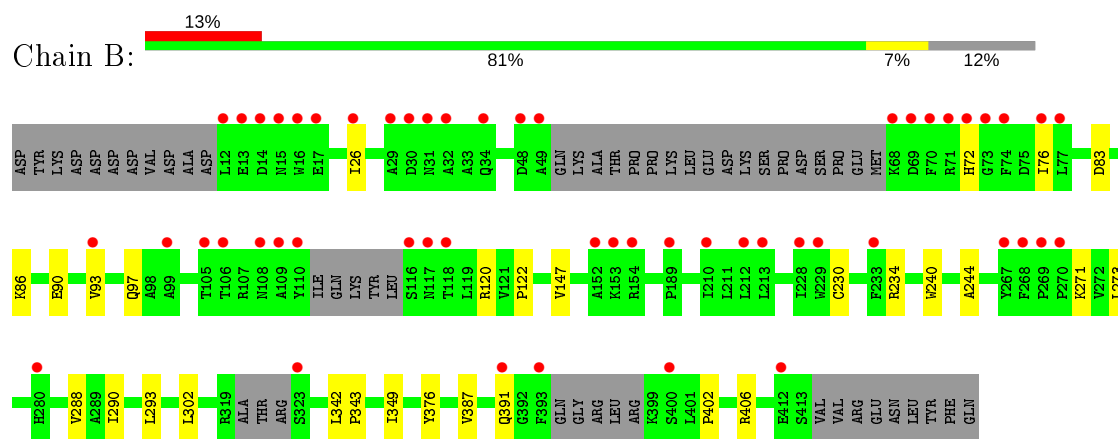


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		
8	B	1	Total	C	O	0	0
			20	18	2		

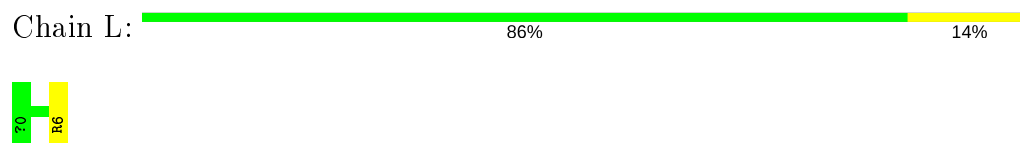
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	39	Total	O	0	0
			39	39		
9	L	6	Total	O	0	0
			6	6		

- Molecule 1: Soluble cytochrome b562, C5a anaphylatoxin chemotactic receptor 1 chimera



- Molecule 2: PMX53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.41Å 52.61Å 83.86Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	27.36 – 2.20 27.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.36-2.20) 99.6 (27.36-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.224 0.197 , 0.227	Depositor DCC
R_{free} test set	1264 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, ZAL, OLC, ACE, NA, MLI, ORN, PGE, YCM, EFD

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	B	0.26	0/2830	0.41	0/3875
2	L	0.29	0/45	0.35	0/57
All	All	0.26	0/2875	0.40	0/3932

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	B	2781	0	2803	18	0
2	L	65	0	64	0	0
3	B	42	0	0	1	0
4	B	14	0	4	0	0
5	B	1	0	0	0	0
6	B	9	0	11	0	0
7	B	50	0	80	3	0
8	B	80	0	132	6	0
9	B	39	0	0	0	0
9	L	6	0	0	0	0
All	All	3087	0	3094	22	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 (22) 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:B:230:YCM:HD2	1:B:234:ARG:HD2	1.69	0.73
1:B:293:LEU:HD22	1:B:349:ILE:HG13	1.73	0.68
1:B:120:ARG:HB3	1:B:122:PRO:HD2	1.79	0.63
1:B:244:ALA:HA	8:B:510:OLA:H122	1.85	0.59
1:B:240:TRP:CD1	8:B:510:OLA:H21	2.38	0.58
1:B:288:VAL:HG22	7:B:506:OLC:H24	1.85	0.58
1:B:147:VAL:HG13	1:B:406:ARG:HG2	1.87	0.56
1:B:302:LEU:HB2	8:B:508:OLA:H141	1.90	0.54
1:B:387:VAL:O	1:B:391:GLN:HG2	2.08	0.53
1:B:290:ILE:HD13	8:B:508:OLA:H21	1.93	0.51
1:B:86:LYS:NZ	1:B:90:GLU:OE2	2.45	0.49
1:B:72:HIS:O	1:B:76:ILE:HG13	2.16	0.46
7:B:507:OLC:H8A	7:B:507:OLC:H11	1.72	0.46
8:B:511:OLA:H61	8:B:511:OLA:H9	1.46	0.45
1:B:402:PRO:O	1:B:406:ARG:HG3	2.18	0.44
7:B:507:OLC:H7A	7:B:507:OLC:H4	1.65	0.44
1:B:342:LEU:HB3	1:B:343:PRO:HD3	2.00	0.43
3:B:501:EFD:C23	3:B:501:EFD:C20	2.96	0.43
1:B:26:ILE:O	1:B:97:GLN:NE2	2.52	0.43
1:B:93:VAL:O	1:B:97:GLN:HG3	2.19	0.43
1:B:240:TRP:CE3	8:B:510:OLA:H9	2.54	0.42
1:B:271:LYS:HE3	1:B:273:LEU:HD21	2.01	0.42

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	B	360/422 (85%)	350 (97%)	10 (3%)	0	100	100
2	L	3/7 (43%)	3 (100%)	0	0	100	100
All	All	363/429 (85%)	353 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	B	281/361 (78%)	279 (99%)	2 (1%)	84	91
2	L	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	285/365 (78%)	282 (99%)	3 (1%)	73	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	ASP
1	B	376	TYR
2	L	6	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ORN	L	2	2	6,7,8	0.53	0	2,7,9	0.18	0
2	ZAL	L	4	2	9,11,12	0.85	0	10,13,15	1.46	2 (20%)
1	YCM	B	230	1	7,9,10	1.08	0	4,10,12	0.53	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	ORN	L	2	2	-	0/5/6/8	-
2	ZAL	L	4	2	-	0/5/14/16	0/1/1/1
1	YCM	B	230	1	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	4	ZAL	C6-C1-C2	2.22	114.76	109.33
2	L	4	ZAL	CB-C1-C6	-2.16	107.04	111.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	230	YCM	SG-CD-CE-NZ2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	230	YCM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	MLI	B	503	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	502	-	0,6,6	0.00	-	0,7,7	0.00	-
8	OLA	B	510	-	16,19,19	0.85	1 (6%)	15,19,19	0.74	0
7	OLC	B	506	-	24,24,24	0.83	1 (4%)	25,25,25	1.33	3 (12%)
8	OLA	B	508	-	16,19,19	0.75	1 (6%)	15,19,19	1.15	0
8	OLA	B	509	-	16,19,19	0.81	1 (6%)	15,19,19	0.84	0
3	EFD	B	501	-	46,46,46	3.26	9 (19%)	62,67,67	1.16	4 (6%)
7	OLC	B	507	-	24,24,24	0.90	1 (4%)	25,25,25	1.25	3 (12%)
8	OLA	B	511	-	16,19,19	0.79	1 (6%)	15,19,19	1.16	0
6	PGE	B	505	-	8,8,9	0.35	0	7,7,8	0.33	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	MLI	B	503	-	-	0/0/4/4	-
4	MLI	B	502	-	-	0/0/4/4	-
8	OLA	B	510	-	-	9/15/17/17	-
7	OLC	B	506	-	-	14/24/24/24	-
8	OLA	B	508	-	-	11/15/17/17	-
8	OLA	B	509	-	-	10/15/17/17	-
3	EFD	B	501	-	-	2/30/51/51	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	B	507	-	-	12/24/24/24	-
8	OLA	B	511	-	-	6/15/17/17	-
6	PGE	B	505	-	-	2/6/6/7	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	EFD	C14-C11	-13.62	1.40	1.54
3	B	501	EFD	C11-N09	-10.53	1.37	1.47
3	B	501	EFD	C13-C14	-8.60	1.37	1.53
3	B	501	EFD	C12-C13	-5.78	1.38	1.53
3	B	501	EFD	C10-N09	-5.66	1.37	1.47
7	B	507	OLC	O20-C1	4.01	1.45	1.33
3	B	501	EFD	C07-N09	3.86	1.43	1.34
7	B	506	OLC	O20-C1	3.54	1.43	1.33
3	B	501	EFD	C12-C10	-3.21	1.40	1.51
3	B	501	EFD	C23-N31	3.17	1.42	1.35
8	B	510	OLA	C10-C9	3.01	1.49	1.31
8	B	508	OLA	C10-C9	2.86	1.48	1.31
8	B	511	OLA	C10-C9	2.82	1.48	1.31
8	B	509	OLA	C10-C9	2.82	1.48	1.31
3	B	501	EFD	C18-N24	2.04	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	506	OLC	O20-C1-C2	3.68	123.44	111.91
7	B	506	OLC	O20-C1-O19	-3.47	114.83	123.59
3	B	501	EFD	C14-C23-N31	2.88	118.04	114.50
3	B	501	EFD	C38-C35-C34	-2.77	121.31	124.12
7	B	507	OLC	O20-C1-C2	2.63	120.15	111.91
3	B	501	EFD	C06-C07-N09	2.62	121.77	118.17
7	B	507	OLC	O20-C1-O19	-2.29	117.82	123.59
7	B	507	OLC	C14-C15-C16	-2.21	103.20	114.42
7	B	506	OLC	C3-C2-C1	-2.00	106.34	113.62
3	B	501	EFD	F42-C39-C34	-2.00	109.21	112.70

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	510	OLA	C1-C2-C3-C4
7	B	506	OLC	C21-C22-C24-O25
7	B	506	OLC	O20-C21-C22-C24
8	B	509	OLA	C1-C2-C3-C4
7	B	507	OLC	C21-C22-C24-O25
7	B	507	OLC	C1-C2-C3-C4
7	B	506	OLC	O20-C21-C22-O23
7	B	507	OLC	O23-C22-C24-O25
7	B	506	OLC	C1-C2-C3-C4
8	B	511	OLA	C11-C12-C13-C14
8	B	511	OLA	C6-C7-C8-C9
8	B	508	OLA	C14-C15-C16-C17
7	B	506	OLC	C3-C4-C5-C6
7	B	506	OLC	C2-C3-C4-C5
8	B	509	OLA	C11-C12-C13-C14
7	B	507	OLC	C13-C14-C15-C16
8	B	508	OLA	C13-C14-C15-C16
8	B	508	OLA	C12-C13-C14-C15
8	B	509	OLA	C5-C6-C7-C8
7	B	506	OLC	O23-C22-C24-O25
8	B	510	OLA	C4-C5-C6-C7
7	B	506	OLC	C14-C15-C16-C17
7	B	507	OLC	C2-C3-C4-C5
7	B	507	OLC	C2-C1-O20-C21
7	B	507	OLC	C3-C4-C5-C6
8	B	509	OLA	C10-C11-C12-C13
8	B	509	OLA	C4-C5-C6-C7
7	B	506	OLC	C12-C13-C14-C15
7	B	507	OLC	O19-C1-O20-C21
8	B	508	OLA	C11-C10-C9-C8
8	B	509	OLA	C12-C13-C14-C15
8	B	510	OLA	C12-C13-C14-C15
8	B	508	OLA	C6-C7-C8-C9
8	B	510	OLA	C5-C6-C7-C8
7	B	507	OLC	C12-C13-C14-C15
3	B	501	EFD	C11-C14-C23-O30
8	B	510	OLA	C10-C11-C12-C13
3	B	501	EFD	C11-C14-C23-N31
7	B	506	OLC	C2-C1-O20-C21
8	B	509	OLA	C6-C7-C8-C9
8	B	508	OLA	C15-C16-C17-C18
6	B	505	PGE	C3-C4-O3-C5
8	B	509	OLA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
7	B	506	OLC	O19-C1-O20-C21
8	B	509	OLA	C15-C16-C17-C18
8	B	508	OLA	C2-C3-C4-C5
8	B	508	OLA	C4-C5-C6-C7
8	B	510	OLA	C11-C10-C9-C8
8	B	511	OLA	C11-C10-C9-C8
8	B	510	OLA	C3-C4-C5-C6
7	B	506	OLC	C7-C8-C9-C10
8	B	508	OLA	C7-C8-C9-C10
7	B	507	OLC	C6-C7-C8-C9
7	B	506	OLC	C6-C7-C8-C9
7	B	507	OLC	C10-C11-C12-C13
6	B	505	PGE	O2-C3-C4-O3
8	B	508	OLA	C5-C6-C7-C8
8	B	511	OLA	C9-C10-C11-C12
7	B	506	OLC	C15-C16-C17-C18
8	B	510	OLA	C9-C10-C11-C12
7	B	507	OLC	C9-C10-C11-C12
8	B	510	OLA	C7-C8-C9-C10
8	B	511	OLA	C15-C16-C17-C18
8	B	511	OLA	C7-C8-C9-C10
8	B	508	OLA	C9-C10-C11-C12
8	B	509	OLA	C7-C8-C9-C10

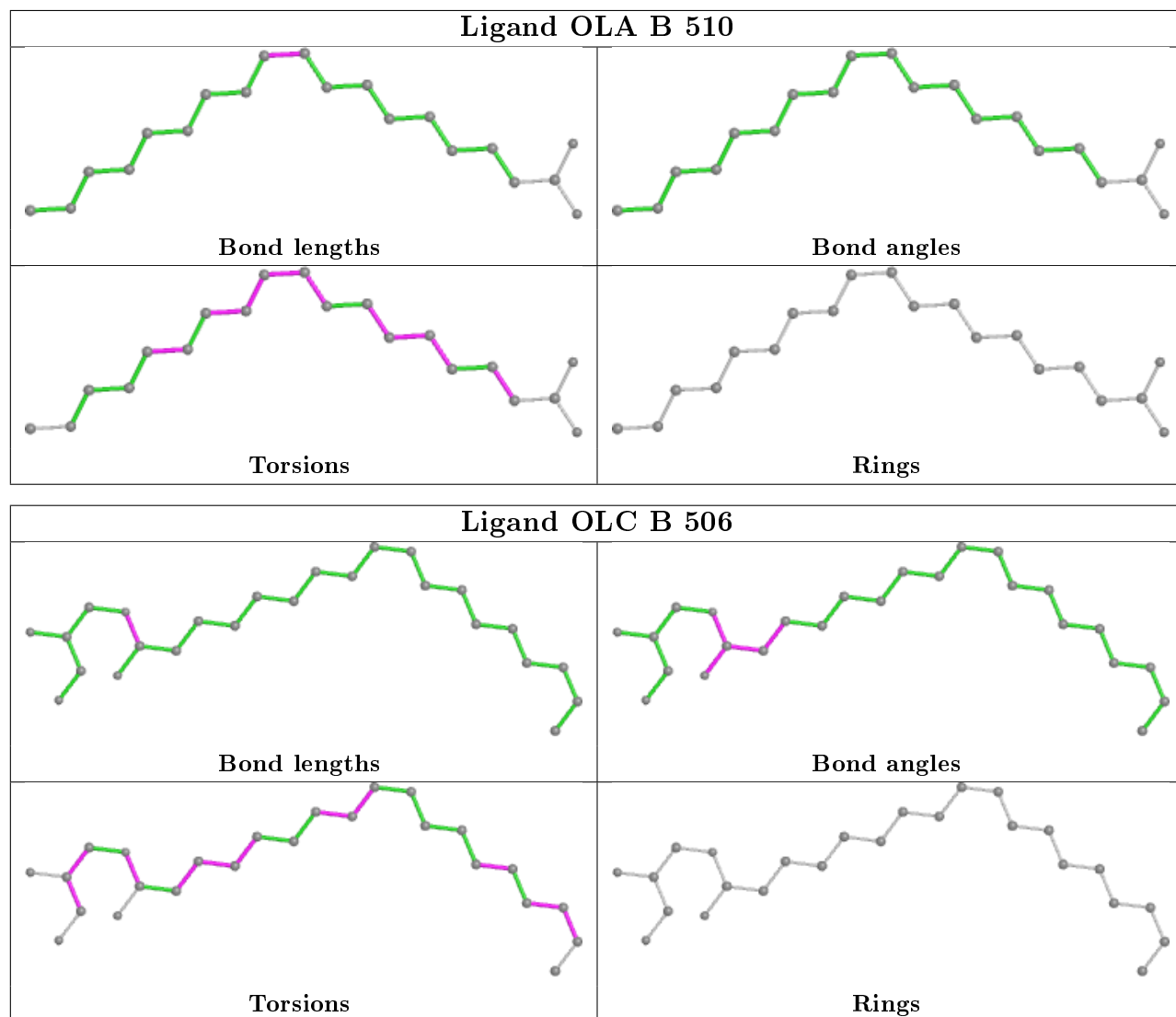
There are no ring outliers.

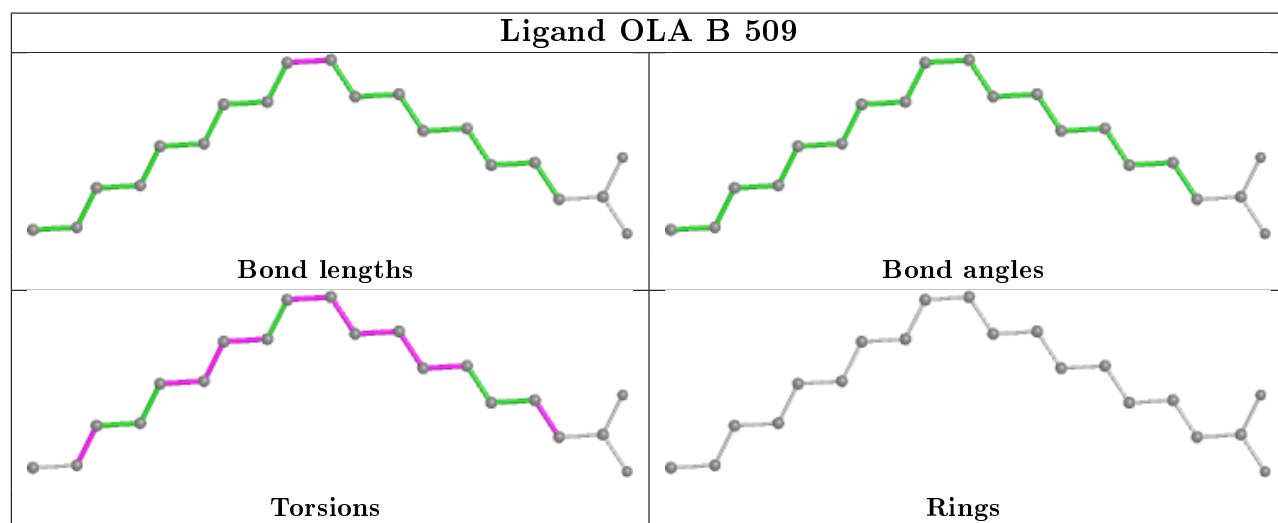
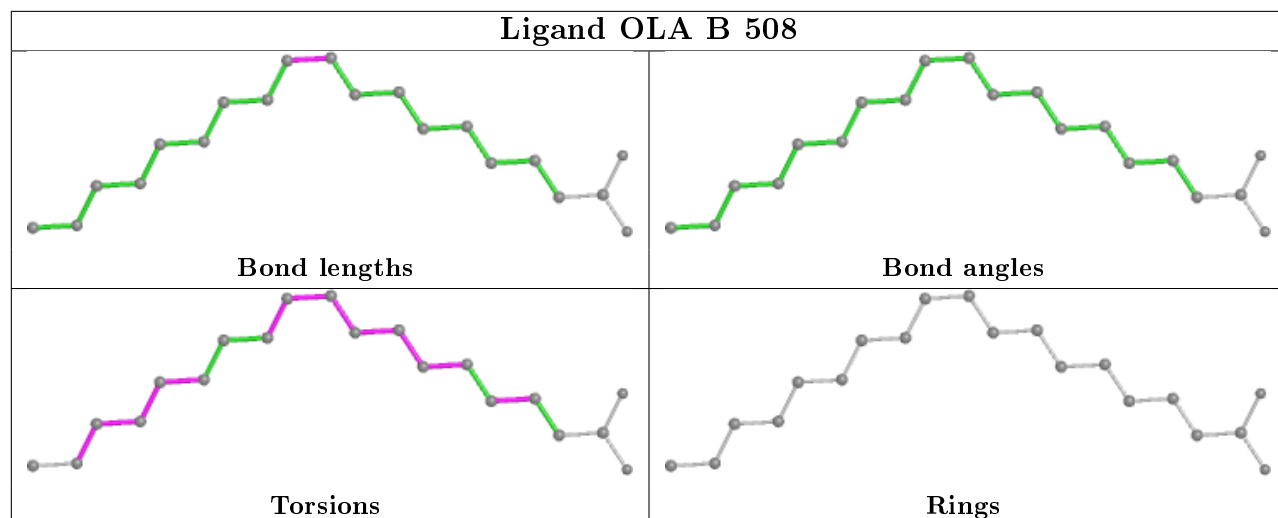
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	510	OLA	3	0
7	B	506	OLC	1	0
8	B	508	OLA	2	0
3	B	501	EFD	1	0
7	B	507	OLC	2	0
8	B	511	OLA	1	0

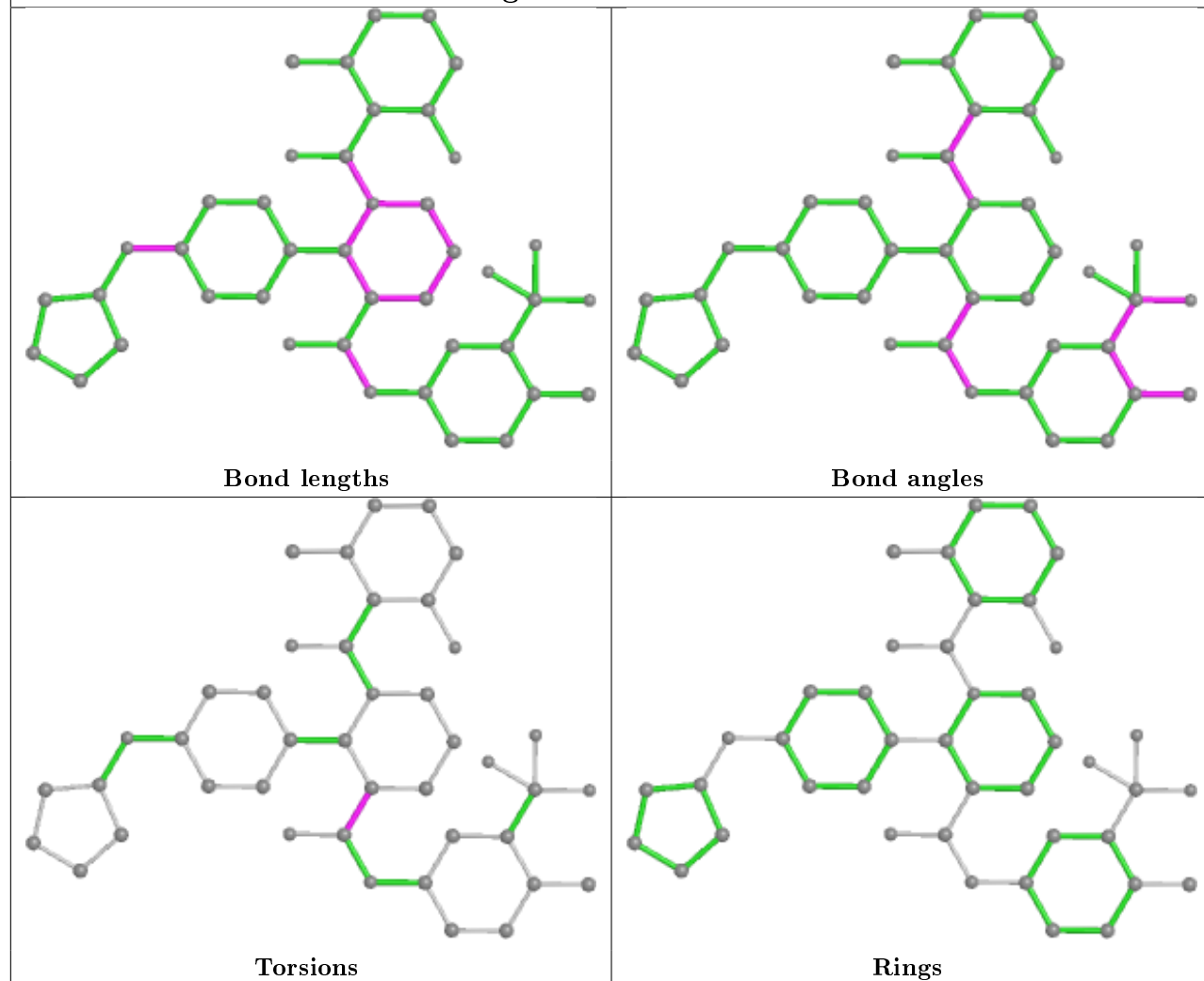
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

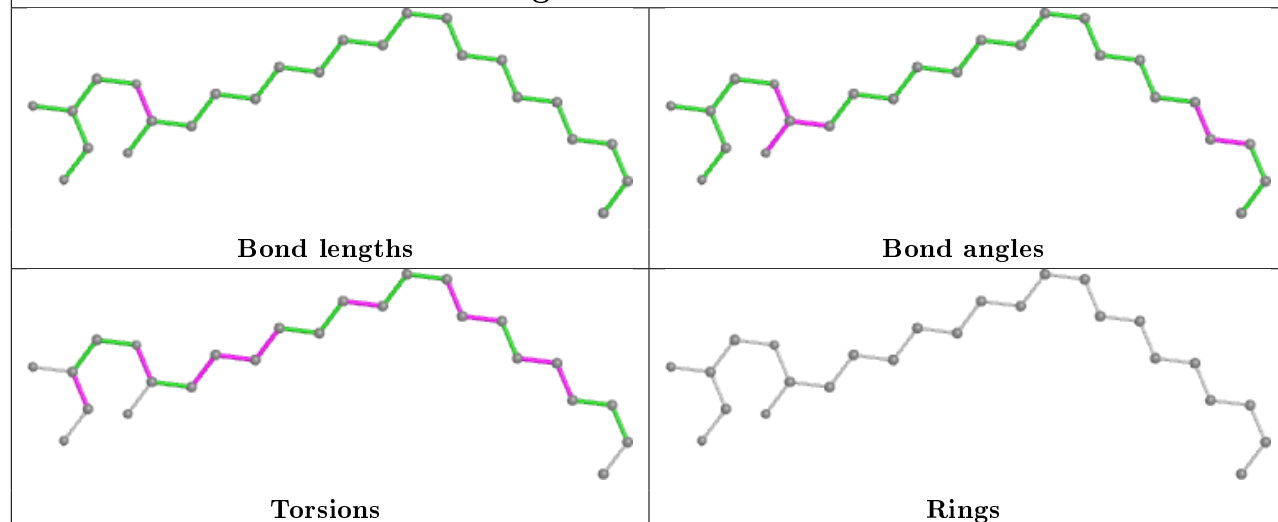


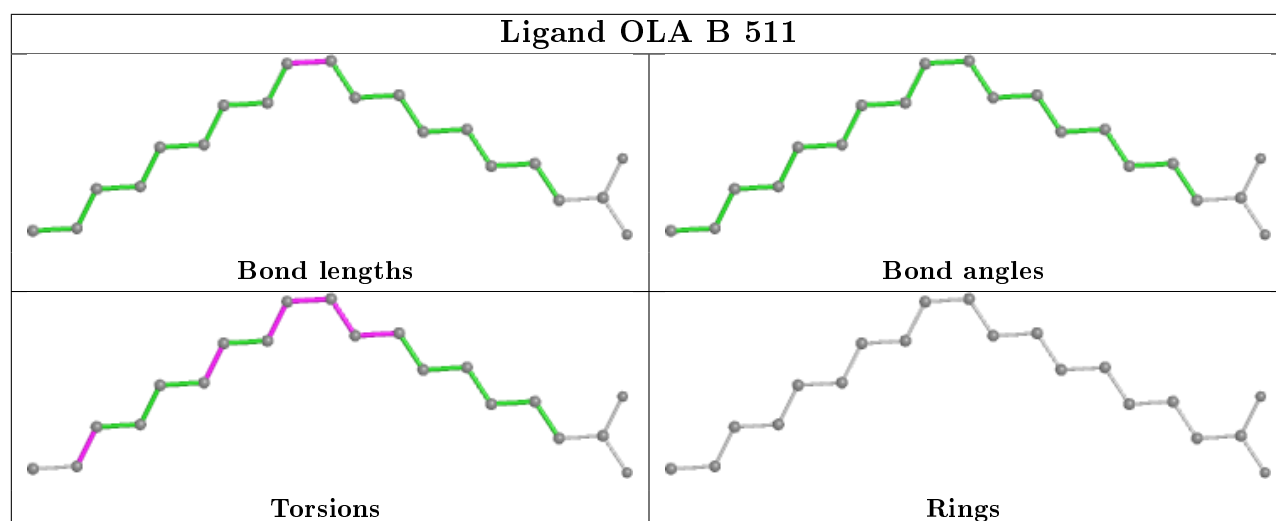


Ligand EFD B 501



Ligand OLC B 507





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	B	370/422 (87%)	0.64	53 (14%) 2 2	23, 44, 94, 113	0
2	L	4/7 (57%)	0.34	0 100 100	33, 39, 39, 40	0
All	All	374/429 (87%)	0.63	53 (14%) 2 2	23, 43, 94, 113	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	PHE	8.2
1	B	29	ALA	5.8
1	B	280	HIS	5.6
1	B	14	ASP	5.5
1	B	31	ASN	5.5
1	B	109	ALA	5.4
1	B	105	THR	5.3
1	B	12	LEU	5.0
1	B	30	ASP	4.9
1	B	72	HIS	4.8
1	B	48	ASP	4.3
1	B	68	LYS	4.3
1	B	15	ASN	4.1
1	B	323	SER	4.0
1	B	228	ILE	3.9
1	B	106	THR	3.8
1	B	76	ILE	3.8
1	B	269	PRO	3.6
1	B	93	VAL	3.5
1	B	267	TYR	3.5
1	B	116	SER	3.5
1	B	34	GLN	3.4
1	B	118	THR	3.3
1	B	77	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	270	PRO	3.2
1	B	73	GLY	3.1
1	B	49	ALA	3.1
1	B	210	ILE	3.0
1	B	268	PHE	3.0
1	B	117	ASN	2.9
1	B	13	GLU	2.8
1	B	17	GLU	2.8
1	B	233	PHE	2.7
1	B	412	GLU	2.7
1	B	229	TRP	2.7
1	B	153	LYS	2.6
1	B	74	PHE	2.6
1	B	32	ALA	2.5
1	B	69	ASP	2.5
1	B	391	GLN	2.5
1	B	108	ASN	2.5
1	B	189	PRO	2.4
1	B	212	LEU	2.4
1	B	393	PHE	2.3
1	B	400	SER	2.3
1	B	154	ARG	2.2
1	B	110	TYR	2.1
1	B	26	ILE	2.1
1	B	213	LEU	2.1
1	B	99	ALA	2.1
1	B	152	ALA	2.1
1	B	71	ARG	2.0
1	B	16	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	YCM	B	230	10/11	0.88	0.15	53,60,69,76	0
2	ORN	L	2	8/9	0.93	0.15	36,37,42,42	0
2	ZAL	L	4	11/12	0.97	0.23	30,37,44,45	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

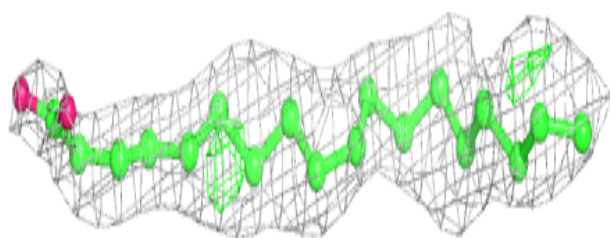
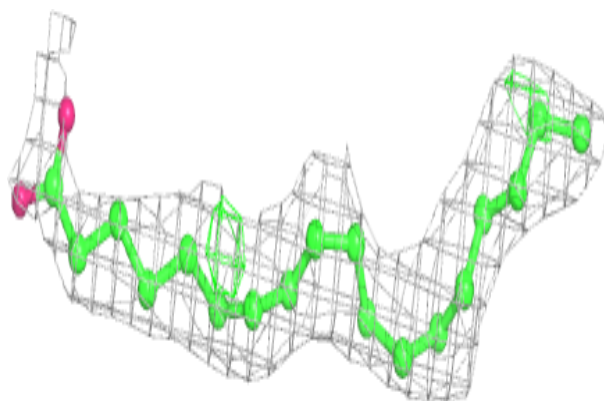
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	OLA	B	509	20/20	0.61	0.22	60,65,79,81	0
8	OLA	B	510	20/20	0.69	0.23	47,61,83,83	0
7	OLC	B	507	25/25	0.74	0.28	59,64,78,78	0
8	OLA	B	511	20/20	0.80	0.26	63,67,78,80	0
4	MLI	B	502	7/7	0.81	0.22	77,79,82,86	0
8	OLA	B	508	20/20	0.83	0.23	39,53,81,81	0
7	OLC	B	506	25/25	0.83	0.18	52,58,75,78	0
6	PGE	B	505	9/10	0.84	0.38	73,75,78,79	0
5	NA	B	504	1/1	0.91	0.10	43,43,43,43	0
4	MLI	B	503	7/7	0.91	0.18	37,51,70,71	0
3	EFD	B	501	42/42	0.93	0.12	33,37,41,45	0

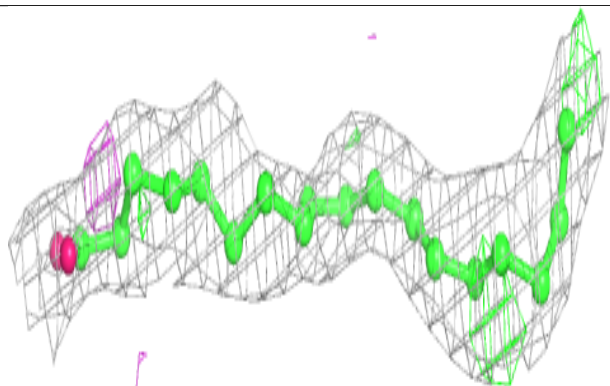
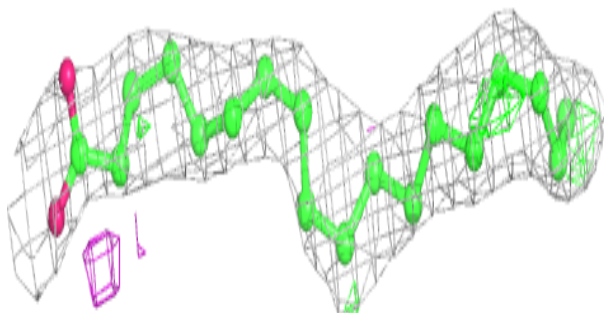
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 509:

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

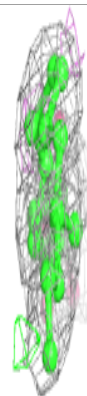
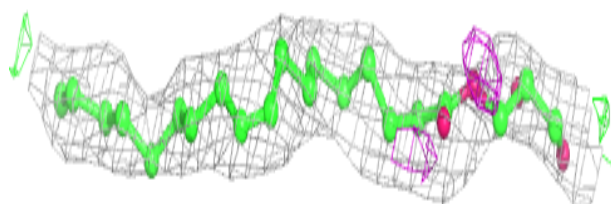
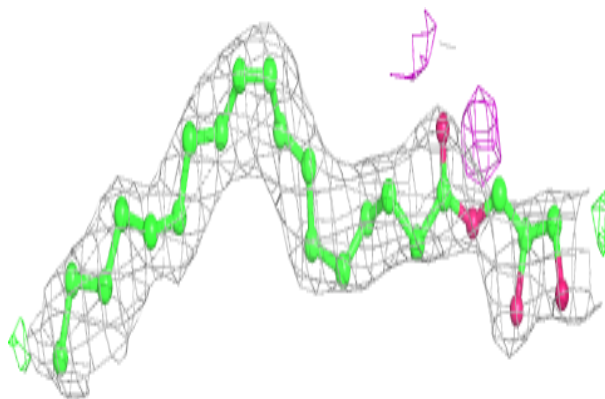
**Electron density around OLA B 510:**

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

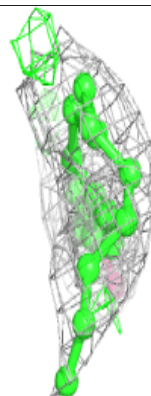
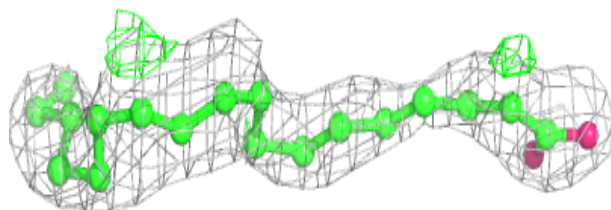
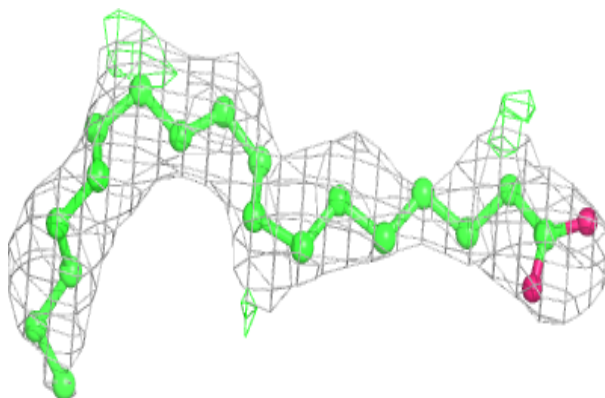


Electron density around OLC B 507:

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

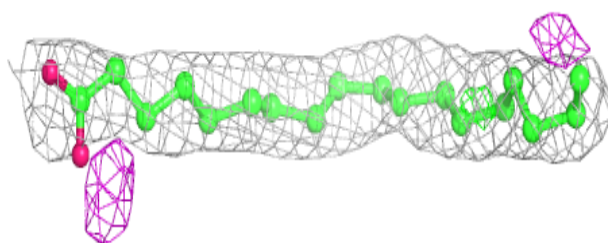
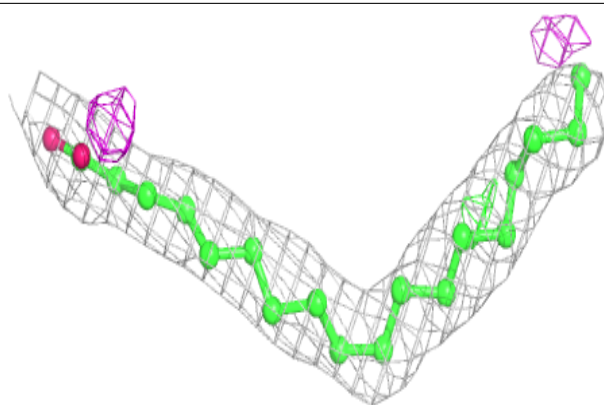
**Electron density around OLA B 511:**

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

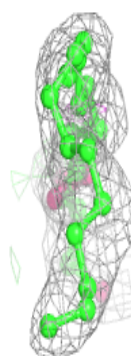
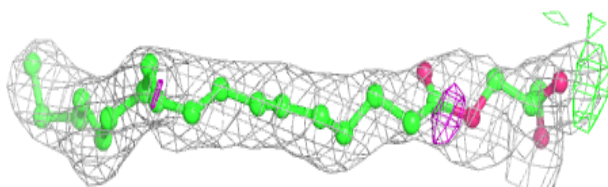
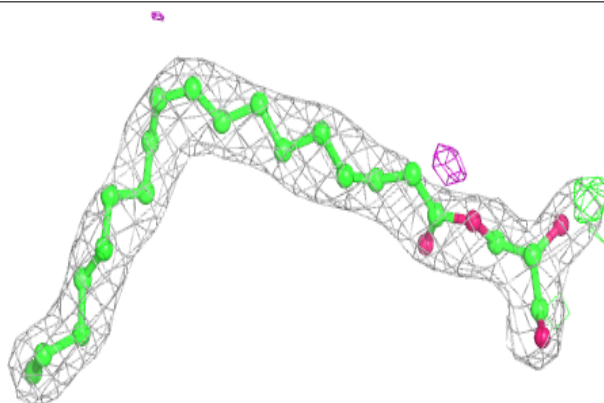


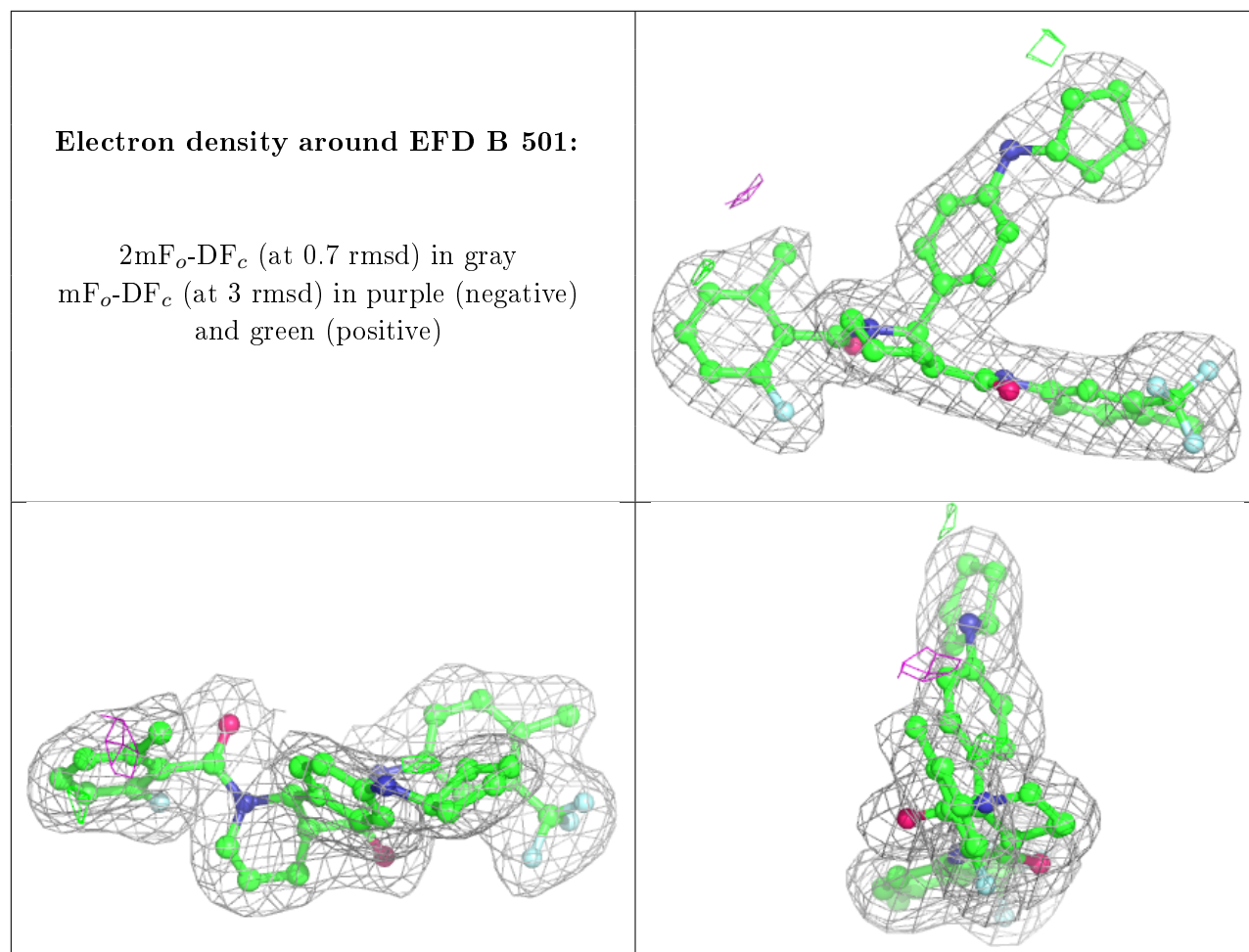
Electron density around OLA B 508:

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

**Electron density around OLC B 506:**

$2mF_o-DF_c$ (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.