



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 5ZKQ / pdb_00005zkq
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

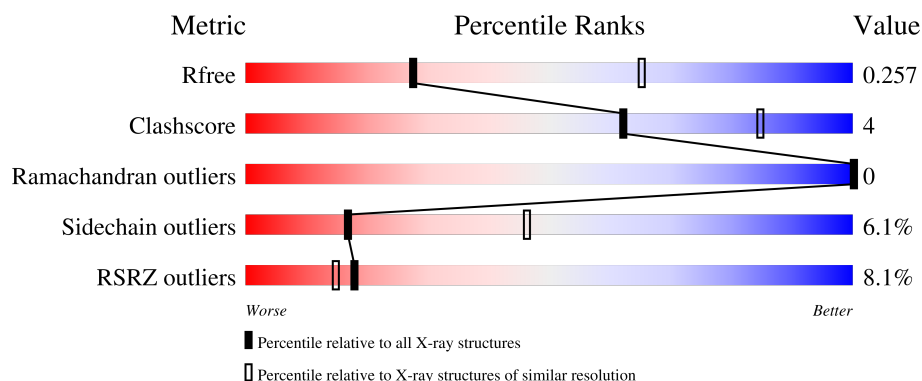
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	438	5% 54% 9% • 36%
1	B	438	7% 74% 16% • 9%

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,Platelet-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:

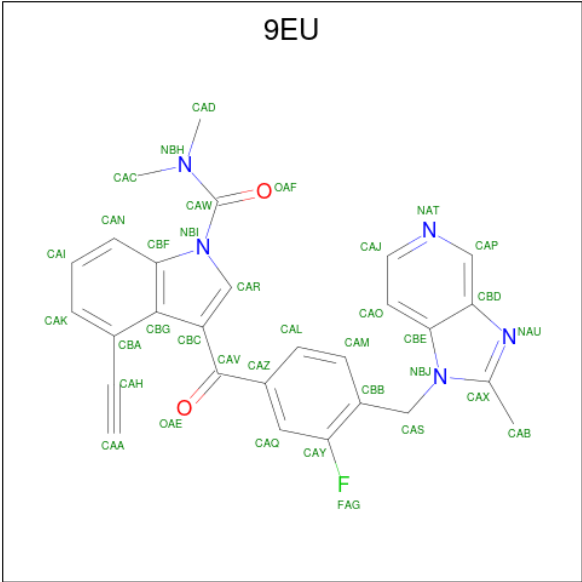
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P25105
A	0	ALA	-	expression tag	UNP P25105
A	1	PRO	-	expression tag	UNP P25105
A	116	TYR	PHE	engineered mutation	UNP P25105
A	169	ASP	ASN	engineered mutation	UNP P25105
A	1011	GLY	-	linker	UNP P00720
A	1012	GLY	-	linker	UNP 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

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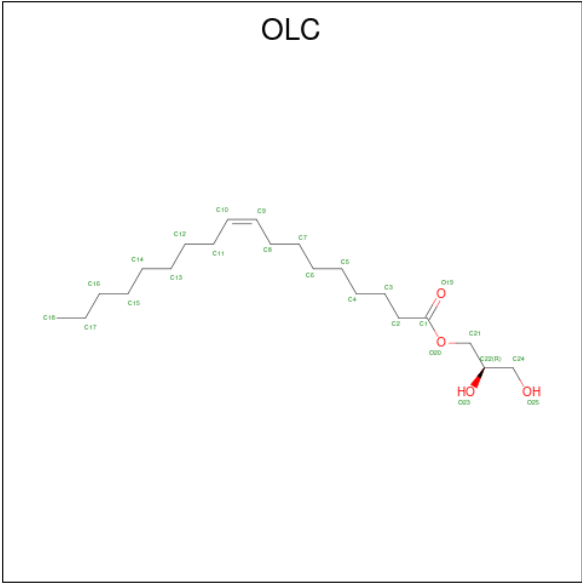
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P25105
B	0	ALA	-	expression tag	UNP P25105
B	1	PRO	-	expression tag	UNP P25105
B	116	TYR	PHE	engineered mutation	UNP P25105
B	169	ASP	ASN	engineered mutation	UNP P25105
B	1011	GLY	-	linker	UNP P00720
B	1012	GLY	-	linker	UNP 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 (CCD ID: 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 (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



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

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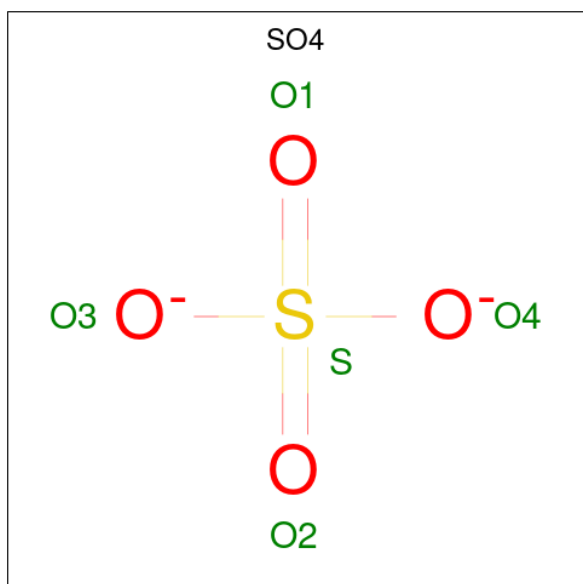
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			12	8	4		
3	B	1	Total	C	O	0	0
			20	16	4		
3	B	1	Total	C	O	0	0
			18	14	4		
3	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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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		

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 49.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.39-2.90) 99.3 (49.39-2.90)	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 , 56.6	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	0.86	1/2238 (0.0%)	1.44	10/3065 (0.3%)
1	B	0.87	0/3219	1.48	20/4390 (0.5%)
All	All	0.87	1/5457 (0.0%)	1.47	30/7455 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	VAL	CA-C	5.64	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	13	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	12	GLU	CA-C-N	6.53	129.35	120.54
1	A	12	GLU	C-N-CA	6.53	129.35	120.54
1	A	262	PHE	CA-CB-CG	6.41	120.21	113.80
1	B	264	ASP	CA-C-N	5.84	128.11	120.28
1	B	264	ASP	C-N-CA	5.84	128.11	120.28
1	B	103	CYS	N-CA-C	-5.64	105.22	111.36
1	A	163	ASP	CA-C-N	5.61	128.06	120.38
1	A	163	ASP	C-N-CA	5.61	128.06	120.38
1	B	250	VAL	CA-C-N	5.46	129.09	120.47
1	B	250	VAL	C-N-CA	5.46	129.09	120.47
1	B	1093	ARG	CA-C-N	5.44	127.89	120.54
1	B	1093	ARG	C-N-CA	5.44	127.89	120.54
1	B	197	LEU	N-CA-C	-5.36	105.36	111.14
1	B	1026	ASP	CA-C-N	5.34	127.40	120.56
1	B	1026	ASP	C-N-CA	5.34	127.40	120.56
1	B	91	ASN	CA-C-N	5.32	127.27	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASN	C-N-CA	5.32	127.27	120.56
1	B	130	THR	N-CA-C	-5.30	105.68	111.82
1	B	281	LEU	CA-C-N	5.22	127.80	120.28
1	B	281	LEU	C-N-CA	5.22	127.80	120.28
1	A	250	VAL	CA-C-N	5.22	127.61	120.46
1	A	250	VAL	C-N-CA	5.22	127.61	120.46
1	B	94	GLY	CA-C-N	5.09	127.05	120.44
1	B	94	GLY	C-N-CA	5.09	127.05	120.44
1	A	16	THR	CA-C-N	5.07	127.34	120.65
1	A	16	THR	C-N-CA	5.07	127.34	120.65
1	B	169	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	260	LEU	N-CA-C	-5.01	106.59	113.30

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
1:B:226:VAL:HG12	1:B:227:LYS:HG3	1.95	0.49
2:B:1201:9EU:CAR	2:B:1201:9EU:CAC	2.90	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:H7A	3:B:1204:OLC:H4	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:96:LEU:HD23	1:B:99:ILE:HD12	2.00	0.43
1:B:1031:VAL:HA	1:B:1034: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:CAR	2:A:501:9EU:CAC	2.98	0.42
1:B:44:TYR:N	1:B:45:PRO:HD3	2.34	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	219 (94%)	13 (6%)	19	50
1	B	330/384 (86%)	309 (94%)	21 (6%)	16	44
All	All	562/768 (73%)	528 (94%)	34 (6%)	17	47

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	52	ILE
1	A	110	VAL
1	A	136	SER
1	A	137	LEU
1	A	145	ILE
1	A	156	ASP
1	A	216	GLN
1	A	230	ASP
1	A	242	ILE
1	A	256	THR
1	A	272	ASN
1	A	285	ASN
1	B	8	HIS
1	B	36	VAL
1	B	37	LEU
1	B	69	THR
1	B	72	LEU
1	B	82	ASN
1	B	84	ILE
1	B	123	ILE
1	B	135	ILE
1	B	137	LEU
1	B	182	VAL
1	B	200	LEU
1	B	202	ILE
1	B	214	LEU
1	B	1008	ILE
1	B	1024	ASN
1	B	1046	SER
1	B	1080	LYS
1	B	241	PHE
1	B	272	ASN
1	B	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	117	GLN
1	A	216	GLN
1	A	248	HIS
1	B	50	ASN

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Mol	Chain	Res	Type
1	B	91	ASN
1	B	188	HIS
1	B	1024	ASN
1	B	1088	ASN
1	B	248	HIS
1	B	263	GLN
1	B	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	OLC	A	503	-	24,24,24	1.17	1 (4%)	25,25,25	0.74	0
3	OLC	B	1203	-	17,17,24	1.18	1 (5%)	18,18,25	0.81	0
3	OLC	B	1202	-	19,19,24	1.12	1 (5%)	20,20,25	0.78	0
3	OLC	A	504	-	24,24,24	1.25	3 (12%)	25,25,25	0.71	0
3	OLC	A	505	-	11,11,24	0.87	0	12,12,25	0.78	0
3	OLC	B	1204	-	24,24,24	1.07	1 (4%)	25,25,25	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9EU	B	1201	-	40,40,40	2.46	21 (52%)	52,59,59	1.79	10 (19%)
5	SO4	B	1211	-	4,4,4	0.32	0	6,6,6	0.35	0
5	SO4	B	1209	-	4,4,4	0.28	0	6,6,6	0.11	0
2	9EU	A	501	-	40,40,40	2.49	19 (47%)	52,59,59	1.67	8 (15%)
5	SO4	B	1210	-	4,4,4	0.33	0	6,6,6	0.17	0
5	SO4	B	1206	-	4,4,4	0.24	0	6,6,6	0.22	0
5	SO4	B	1207	-	4,4,4	0.30	0	6,6,6	0.34	0
3	OLC	A	502	-	19,19,24	1.15	1 (5%)	20,20,25	0.68	0
5	SO4	B	1208	-	4,4,4	0.26	0	6,6,6	0.17	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	503	-	-	15/24/24/24	-
3	OLC	B	1203	-	-	7/17/17/24	-
3	OLC	B	1202	-	-	11/19/19/24	-
3	OLC	A	504	-	-	15/24/24/24	-
3	OLC	A	505	-	-	7/11/11/24	-
3	OLC	B	1204	-	-	11/24/24/24	-
2	9EU	B	1201	-	-	5/21/22/22	0/5/5/5
2	9EU	A	501	-	-	7/21/22/22	0/5/5/5
3	OLC	A	502	-	-	10/19/19/24	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	9EU	CAS-CBB	-6.73	1.39	1.51
2	A	501	9EU	CAS-CBB	-6.40	1.40	1.51
2	A	501	9EU	CBF-NBI	-4.46	1.34	1.40
3	A	503	OLC	C9-C10	4.43	1.56	1.31
3	A	504	OLC	C9-C10	4.41	1.56	1.31
2	B	1201	9EU	CBG-CBC	-4.30	1.35	1.45
3	B	1204	OLC	C9-C10	4.19	1.55	1.31
3	A	502	OLC	C9-C10	4.14	1.55	1.31
2	B	1201	9EU	CBC-CAV	-4.13	1.35	1.47
2	A	501	9EU	CBG-CBC	-4.09	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	9EU	CBG-CBA	-3.93	1.36	1.41
3	B	1202	OLC	C9-C10	3.92	1.53	1.31
2	A	501	9EU	CBC-CAV	-3.74	1.36	1.47
3	B	1203	OLC	C9-C10	3.67	1.56	1.29
2	A	501	9EU	CAZ-CAV	-3.49	1.42	1.49
2	B	1201	9EU	CBG-CBA	-3.45	1.37	1.41
2	B	1201	9EU	CBF-NBI	-3.44	1.35	1.40
2	A	501	9EU	CAP-CBD	-3.40	1.34	1.39
2	B	1201	9EU	CAZ-CAV	-3.38	1.42	1.49
2	B	1201	9EU	CBD-NAU	-3.37	1.33	1.39
2	B	1201	9EU	CAP-NAT	3.35	1.41	1.34
2	A	501	9EU	CAP-NAT	3.24	1.41	1.34
2	A	501	9EU	CBD-NAU	-3.10	1.33	1.39
2	A	501	9EU	CAN-CBF	-2.96	1.35	1.39
2	A	501	9EU	CAS-NBJ	2.91	1.51	1.46
2	B	1201	9EU	CAP-CBD	-2.88	1.35	1.39
2	A	501	9EU	CAB-CAX	2.86	1.53	1.49
2	B	1201	9EU	CAS-NBJ	2.85	1.51	1.46
2	A	501	9EU	CBG-CBF	-2.84	1.36	1.41
2	A	501	9EU	CBE-CBD	-2.82	1.35	1.40
2	B	1201	9EU	CAJ-NAT	2.81	1.41	1.33
2	A	501	9EU	CAO-CBE	-2.79	1.35	1.39
2	B	1201	9EU	CAN-CBF	-2.70	1.35	1.39
2	A	501	9EU	CAR-NBI	-2.67	1.33	1.38
2	B	1201	9EU	FAG-CAY	-2.66	1.28	1.35
2	B	1201	9EU	CBG-CBF	-2.62	1.36	1.41
2	B	1201	9EU	CBE-NBJ	-2.59	1.34	1.39
2	B	1201	9EU	CAR-NBI	-2.59	1.33	1.38
2	B	1201	9EU	CBE-CBD	-2.56	1.36	1.40
2	A	501	9EU	CBE-NBJ	-2.54	1.35	1.39
2	B	1201	9EU	CAO-CBE	-2.52	1.35	1.39
2	A	501	9EU	CAJ-NAT	2.48	1.40	1.33
2	A	501	9EU	CAR-CBC	-2.46	1.33	1.37
2	B	1201	9EU	CAR-CBC	-2.34	1.33	1.37
2	B	1201	9EU	CAB-CAX	2.33	1.52	1.49
3	A	504	OLC	O20-C1	2.23	1.39	1.33
3	A	504	OLC	C2-C1	2.16	1.57	1.50
2	B	1201	9EU	CAQ-CAY	2.09	1.41	1.37

All (18) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	9EU	NBH-CAW-NBI	6.14	121.02	114.90
2	A	501	9EU	NBH-CAW-NBI	6.02	120.89	114.90
2	B	1201	9EU	CAB-CAX-NBJ	4.23	127.49	123.04
2	B	1201	9EU	CAO-CAJ-NAT	-3.71	117.28	123.60
2	A	501	9EU	CAO-CAJ-NAT	-3.67	117.33	123.60
2	A	501	9EU	CAB-CAX-NBJ	3.37	126.58	123.04
2	B	1201	9EU	CBG-CBC-CAR	3.10	109.09	105.96
2	A	501	9EU	CBD-CBE-NBJ	2.76	107.73	105.55
2	B	1201	9EU	CBG-CBF-NBI	2.72	109.27	107.25
2	B	1201	9EU	CBD-CBE-NBJ	2.68	107.67	105.55
2	B	1201	9EU	CAK-CBA-CAH	-2.58	115.19	119.47
2	A	501	9EU	CAR-CBC-CAV	-2.35	121.17	126.48
2	B	1201	9EU	CAR-CBC-CAV	-2.28	121.32	126.48
2	A	501	9EU	CAK-CBA-CAH	-2.25	115.74	119.47
2	A	501	9EU	CBF-NBI-CAW	2.15	128.17	123.54
2	B	1201	9EU	CBF-NBI-CAR	-2.12	106.66	108.03
2	B	1201	9EU	CAQ-CAY-CBB	-2.06	120.59	123.76
2	A	501	9EU	NBJ-CAX-NAU	-2.00	109.82	112.41

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	9EU	CAZ-CAV-CBC-CAR
2	A	501	9EU	OAE-CAV-CBC-CAR
2	A	501	9EU	OAE-CAV-CBC-CBG
2	B	1201	9EU	CAZ-CAV-CBC-CAR
2	B	1201	9EU	CAZ-CAV-CBC-CBG
2	B	1201	9EU	OAE-CAV-CBC-CAR
2	B	1201	9EU	OAE-CAV-CBC-CBG
3	A	503	OLC	O20-C21-C22-C24
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	B	1202	OLC	C10-C11-C12-C13
3	B	1202	OLC	O20-C21-C22-C24
3	B	1202	OLC	O20-C21-C22-O23
3	A	503	OLC	O19-C1-O20-C21
3	B	1203	OLC	O19-C1-O20-C21
3	A	503	OLC	C2-C1-O20-C21

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

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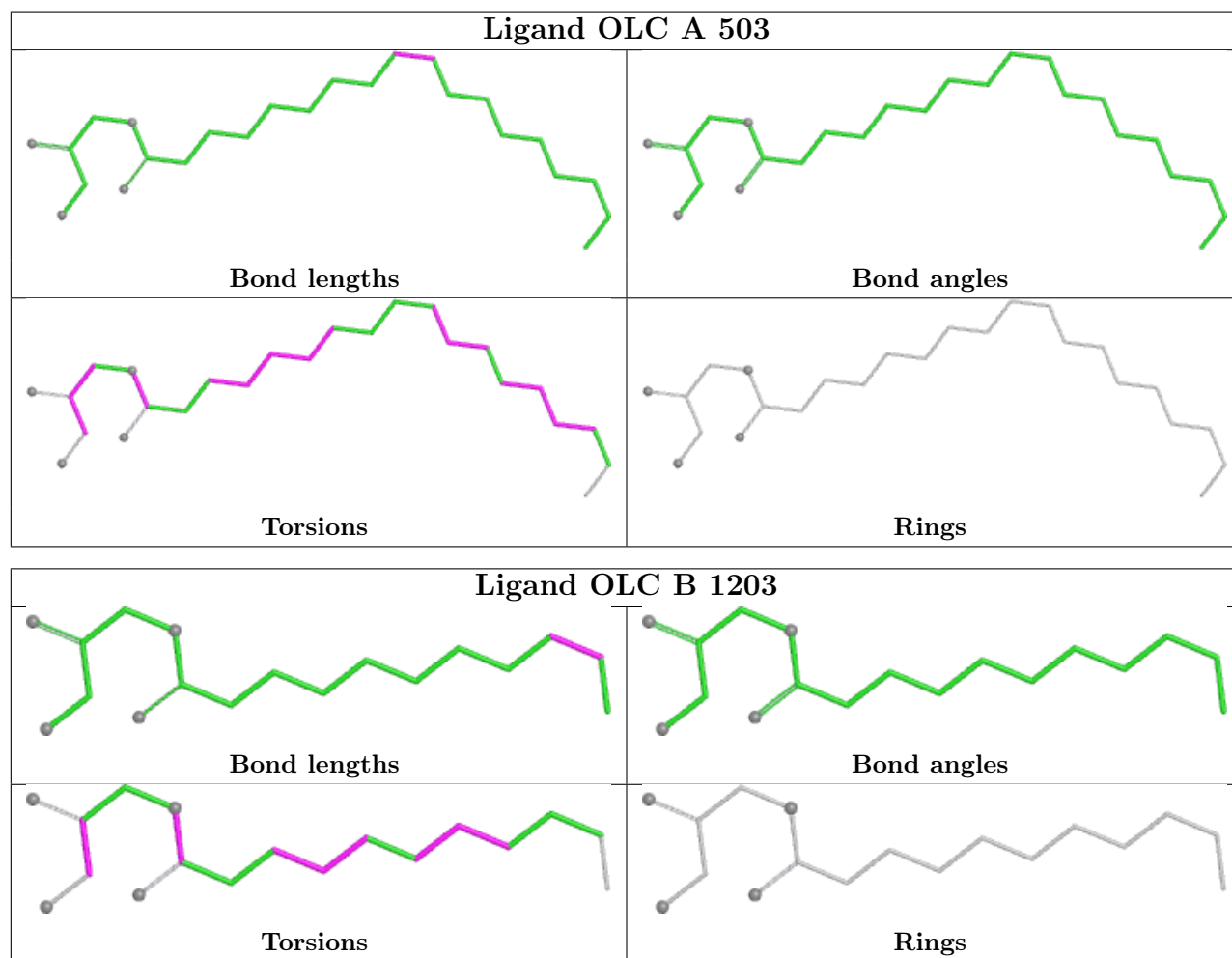
Mol	Chain	Res	Type	Atoms
3	A	505	OLC	O19-C1-O20-C21
3	B	1204	OLC	C2-C3-C4-C5
3	B	1203	OLC	C6-C7-C8-C9
3	A	504	OLC	C1-C2-C3-C4
3	B	1204	OLC	C5-C6-C7-C8
3	B	1203	OLC	C5-C6-C7-C8
3	A	502	OLC	C3-C4-C5-C6
3	B	1202	OLC	O23-C22-C24-O25
3	A	505	OLC	C2-C3-C4-C5
2	A	501	9EU	OAF-CAW-NBI-CAR
3	A	502	OLC	C6-C7-C8-C9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

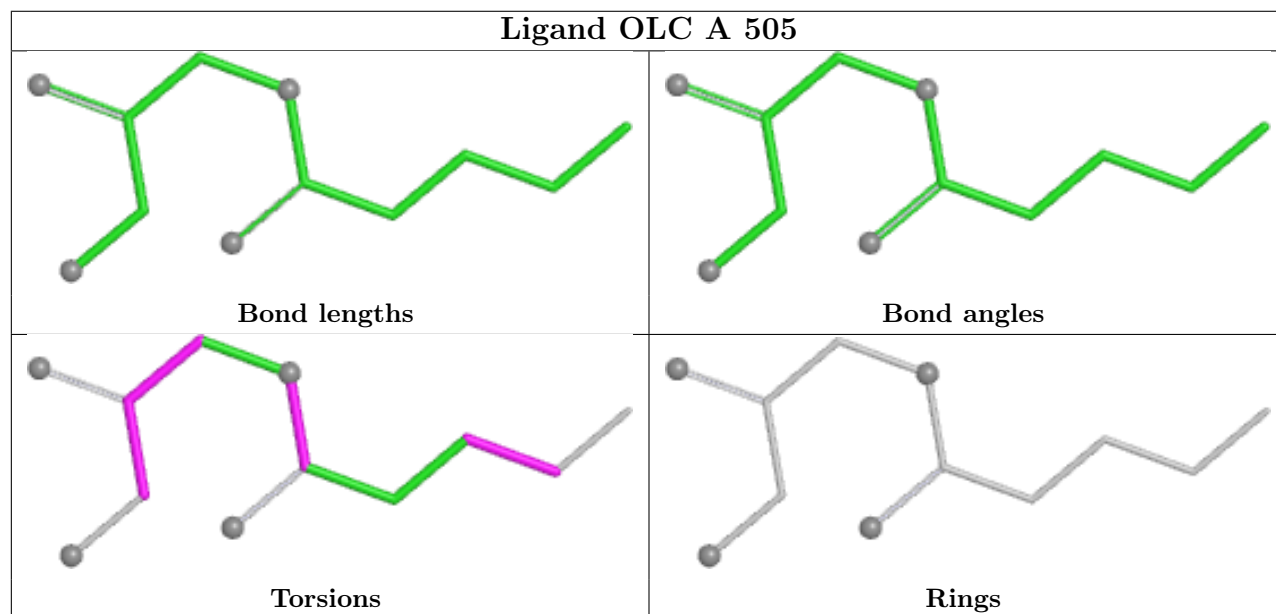
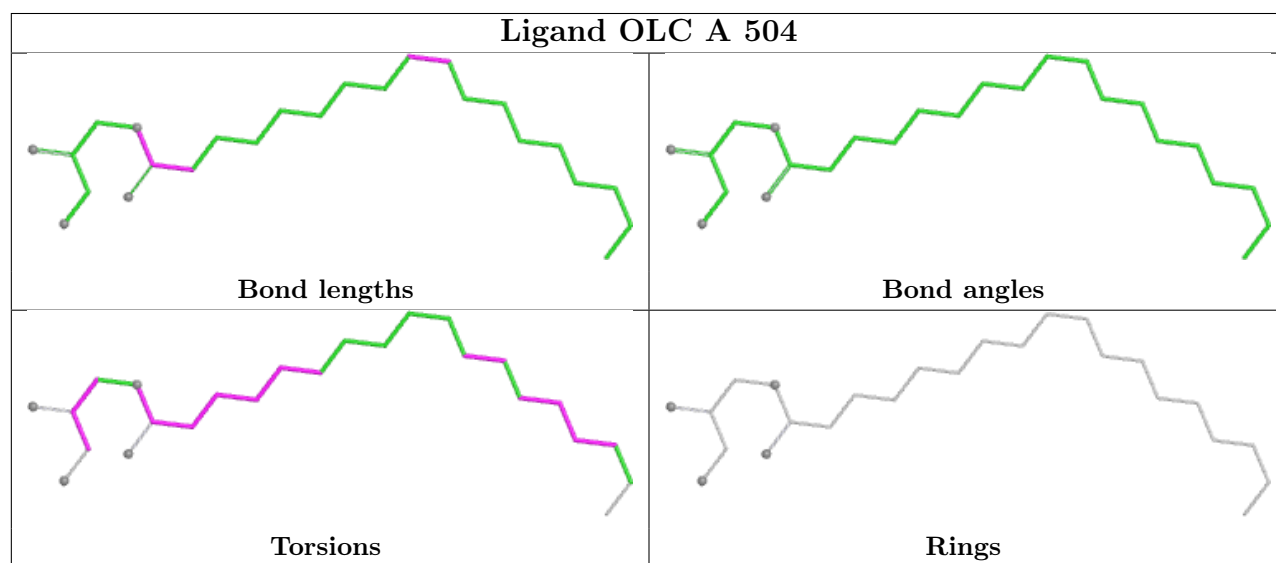
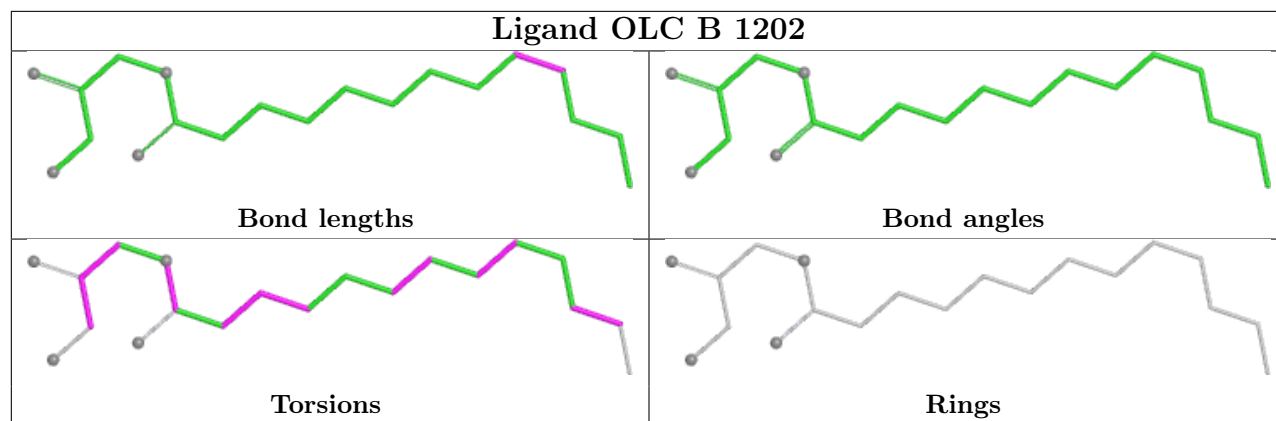
There are no ring outliers.

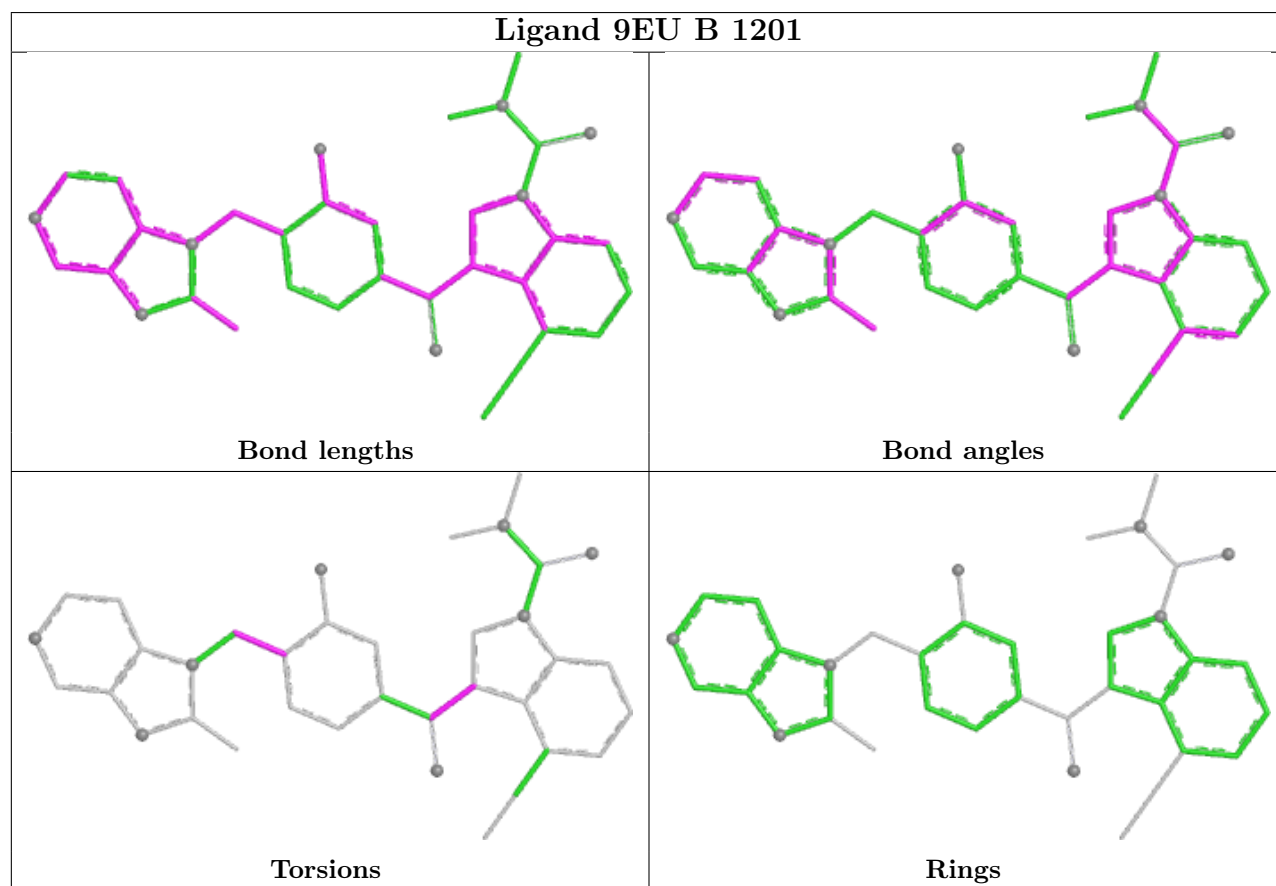
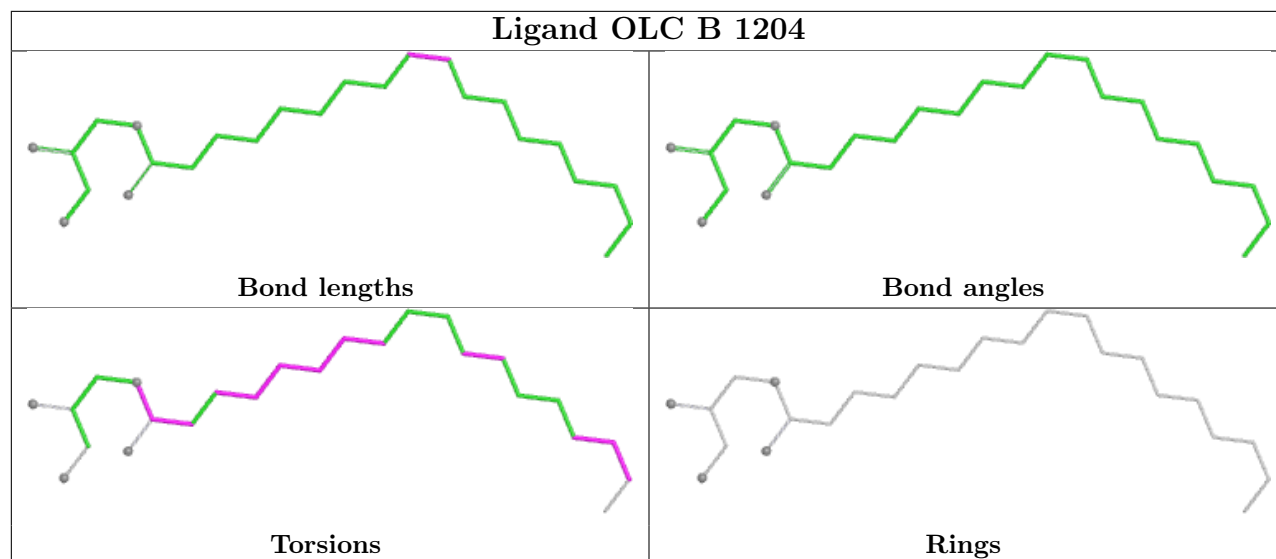
8 monomers are involved in 10 short contacts:

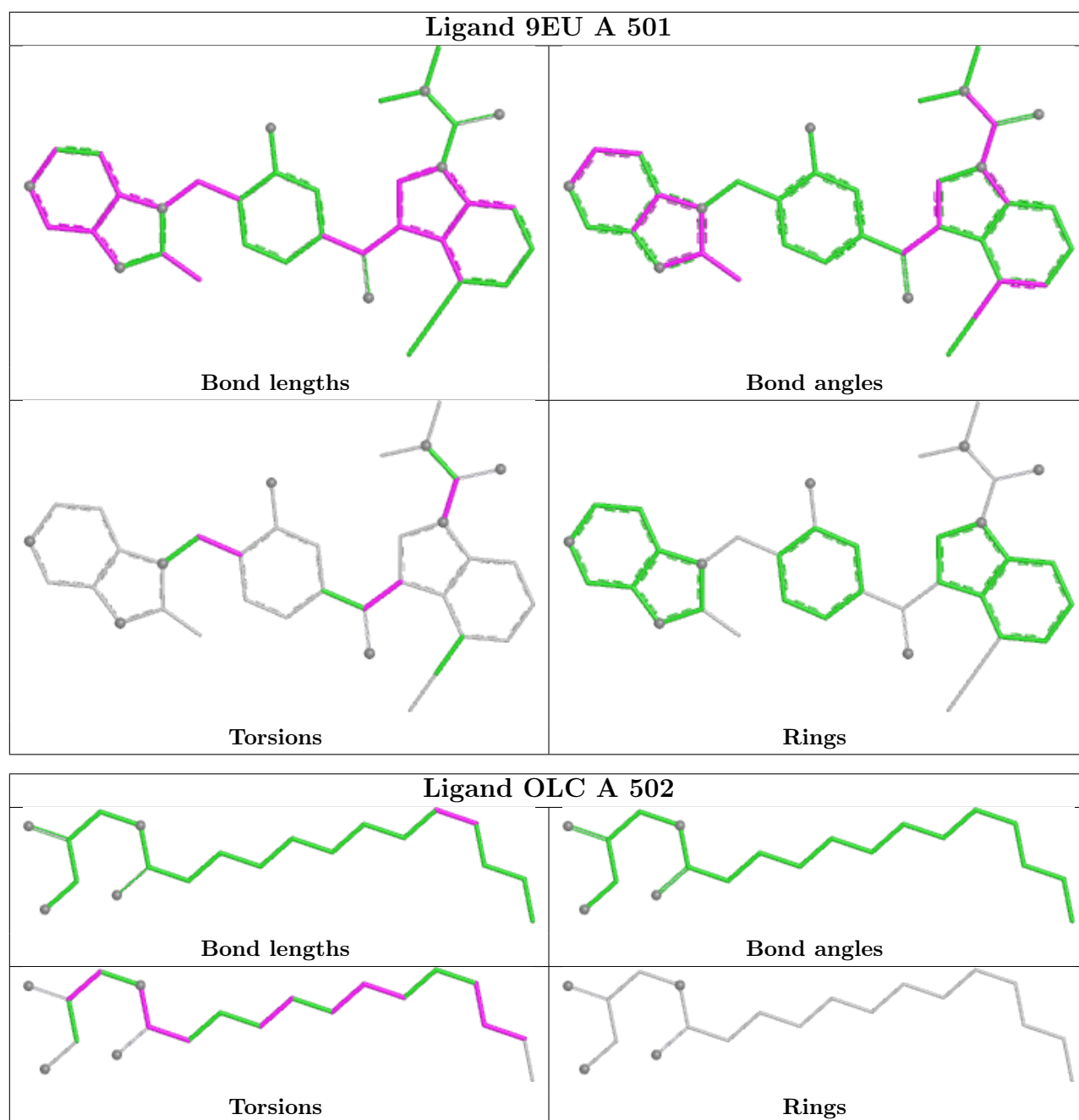
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	OLC	1	0
3	B	1203	OLC	1	0
3	B	1202	OLC	2	0
3	B	1204	OLC	2	0
2	B	1201	9EU	1	0
5	B	1211	SO4	1	0
2	A	501	9EU	1	0
3	A	502	OLC	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/438 (63%)	0.48	24 (8%) 16 13	60, 89, 143, 159	0
1	B	399/438 (91%)	0.30	31 (7%) 19 16	39, 73, 127, 155	1 (0%)
All	All	678/876 (77%)	0.37	55 (8%) 18 15	39, 79, 139, 159	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	SER	5.6
1	B	1018	GLU	4.8
1	A	5	ASP	4.8
1	B	1020	GLU	4.7
1	B	123	ILE	4.4
1	B	128	ALA	4.4
1	B	300	PHE	4.3
1	B	127	GLN	4.3
1	B	117	GLN	3.9
1	B	129	ASN	3.6
1	B	88[A]	PHE	3.6
1	A	128	ALA	3.5
1	A	227	LYS	3.4
1	B	89	LEU	3.4
1	B	49	PHE	3.4
1	A	212	THR	3.3
1	A	11	SER	3.3
1	A	118	ALA	3.3
1	B	39	VAL	3.3
1	B	121	ARG	3.2
1	A	38	TRP	3.2
1	B	45	PRO	3.2
1	B	262	PHE	3.1
1	A	6	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1015	GLY	3.0
1	B	1078	GLN	3.0
1	A	78	GLN	2.9
1	A	39	VAL	2.9
1	A	127	GLN	2.9
1	A	40	PHE	2.9
1	A	8	HIS	2.9
1	B	1004	GLU	2.8
1	B	213	LEU	2.8
1	B	11	SER	2.8
1	A	161	VAL	2.7
1	B	8	HIS	2.6
1	B	1017	ASP	2.6
1	A	49	PHE	2.6
1	B	113	TYR	2.5
1	A	297	THR	2.4
1	A	213	LEU	2.4
1	A	224	ALA	2.4
1	A	217	PRO	2.4
1	B	261	GLY	2.3
1	A	262	PHE	2.3
1	A	9	MET	2.2
1	B	120	THR	2.2
1	A	232	TRP	2.2
1	B	298	LYS	2.2
1	B	1014	SER	2.2
1	B	118	ALA	2.2
1	B	37	LEU	2.1
1	A	7	SER	2.1
1	B	226	VAL	2.0
1	A	230	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

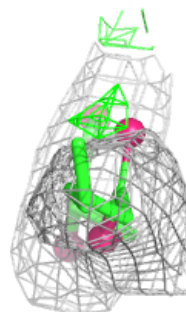
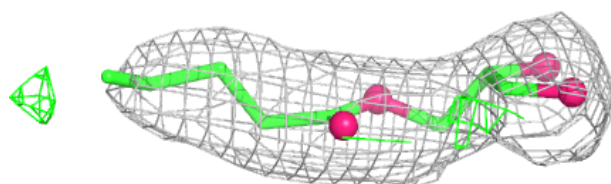
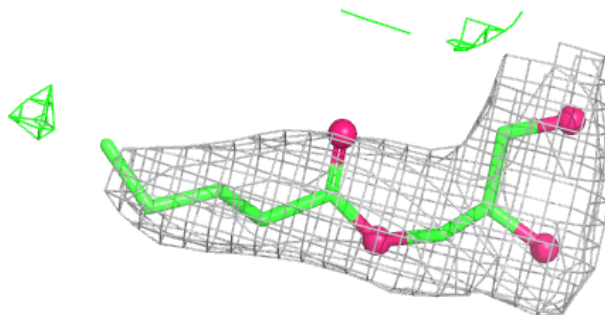
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	1209	5/5	0.77	0.16	172,172,173,173	0
3	OLC	A	505	12/25	0.80	0.19	98,102,103,105	0
3	OLC	A	504	25/25	0.83	0.28	85,96,107,108	0
3	OLC	B	1204	25/25	0.86	0.21	88,97,104,105	0
5	SO4	B	1206	5/5	0.87	0.14	149,149,149,150	0
3	OLC	A	503	25/25	0.87	0.20	69,81,112,112	0
3	OLC	B	1203	18/25	0.88	0.18	88,97,108,109	0
5	SO4	B	1211	5/5	0.91	0.11	101,103,104,105	0
3	OLC	B	1202	20/25	0.94	0.16	76,97,128,129	0
5	SO4	B	1210	5/5	0.94	0.07	90,90,91,92	0
3	OLC	A	502	20/25	0.94	0.17	75,92,117,117	0
4	ZN	B	1205	1/1	0.95	0.09	142,142,142,142	0
2	9EU	B	1201	36/36	0.95	0.10	65,84,92,93	0
5	SO4	B	1208	5/5	0.95	0.12	76,80,81,84	0
5	SO4	B	1207	5/5	0.96	0.09	77,80,82,83	0
2	9EU	A	501	36/36	0.97	0.09	76,82,87,93	0
4	ZN	A	506	1/1	0.98	0.06	121,121,121,121	0

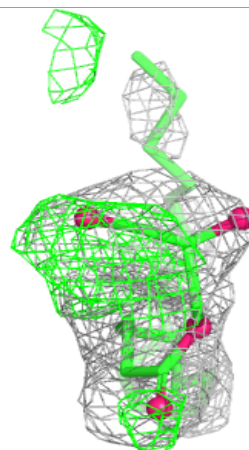
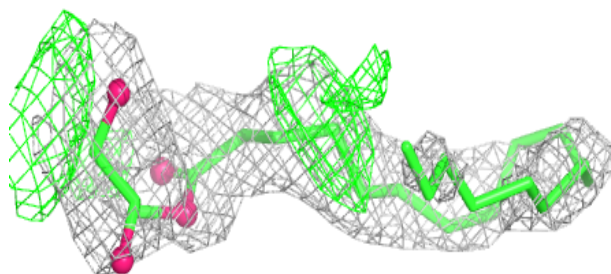
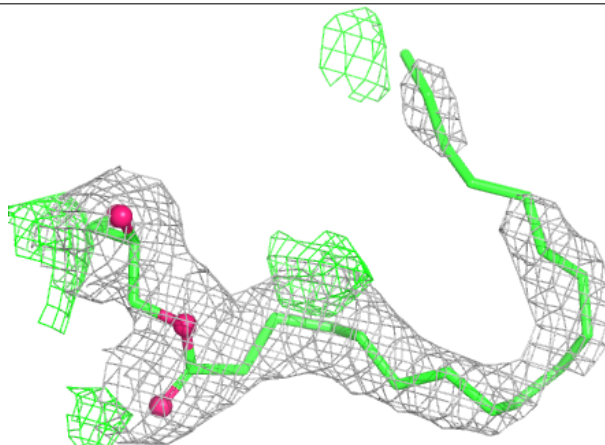
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC 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)

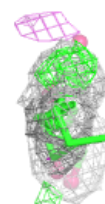
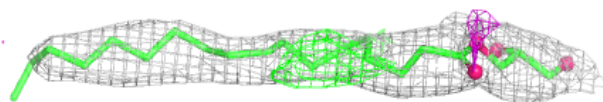
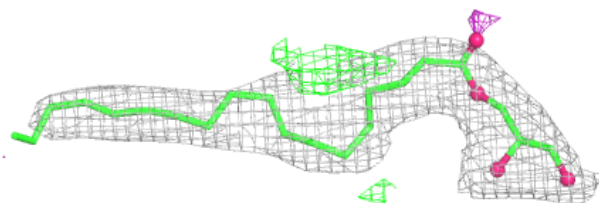
**Electron density around OLC A 504:**

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

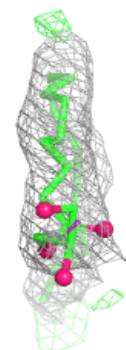
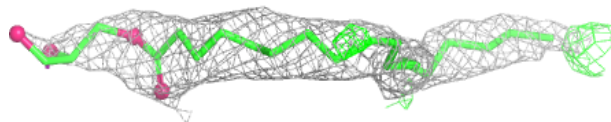
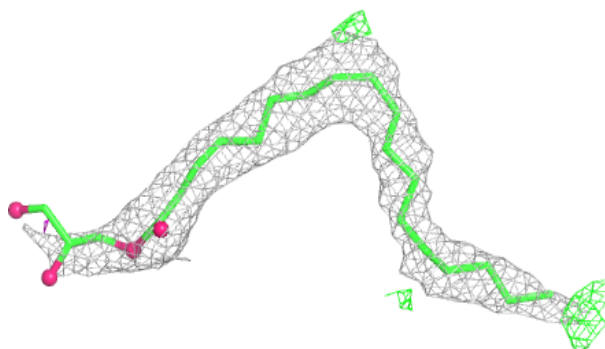


Electron density around OLC B 1204:

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

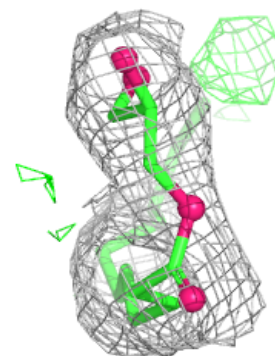
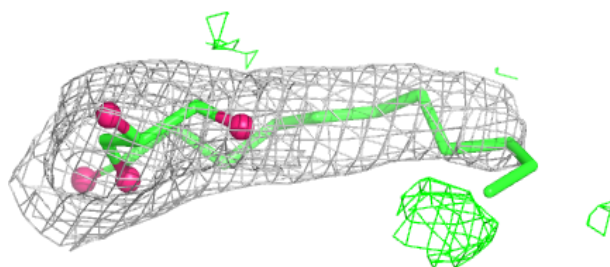
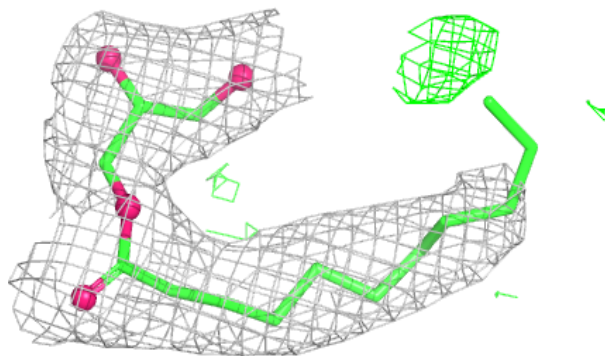
**Electron density around OLC A 503:**

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

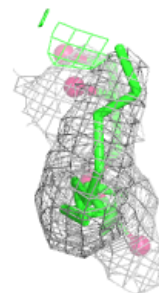
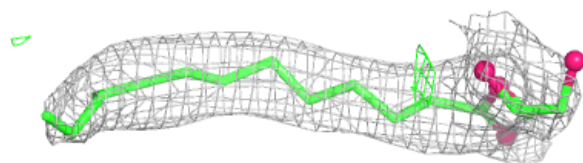
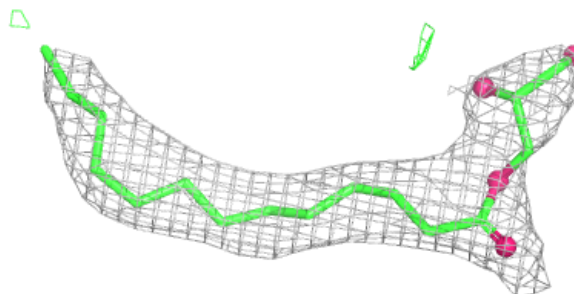


Electron density around OLC B 1203:

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

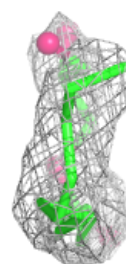
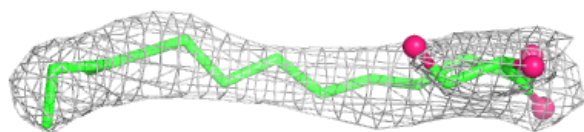
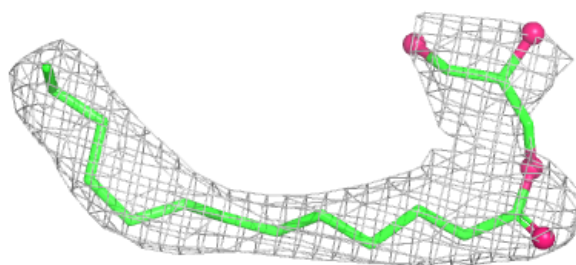
**Electron density around OLC B 1202:**

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

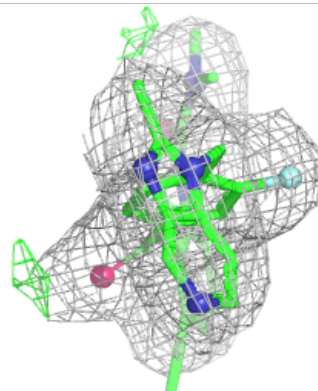
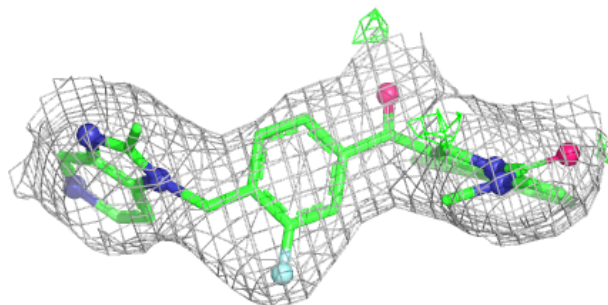
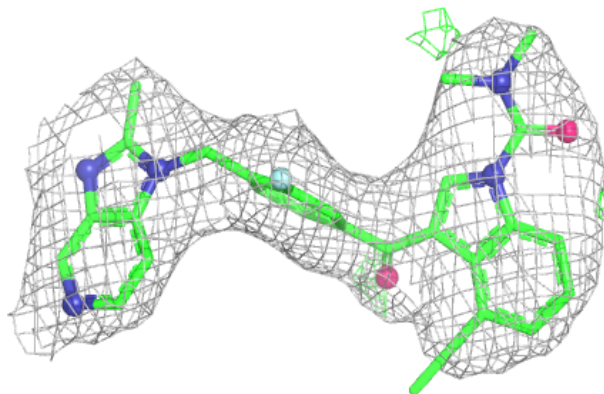


Electron density around OLC A 502:

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

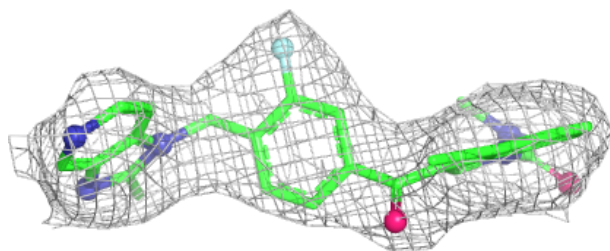
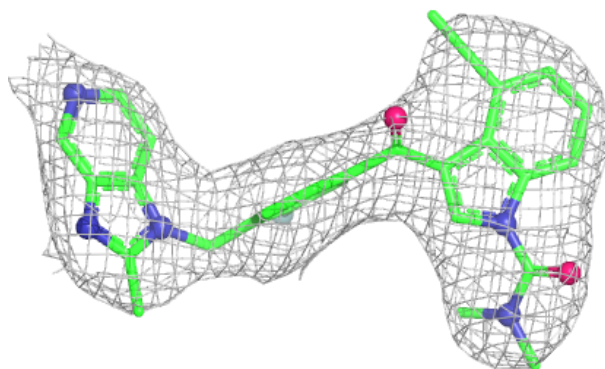
**Electron density around 9EU B 1201:**

$2mF_o-DF_c$ (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.