Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 12:53 PM EDT

PDB ID	:	5TZR
Title	:	GPR40 in complex with partial agonist MK-8666
Authors	:	Lu, J.; Byrne, N.; Patel, S.; Sharma, S.; Soisson, S.M.
Deposited on	:	2016-11-22
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

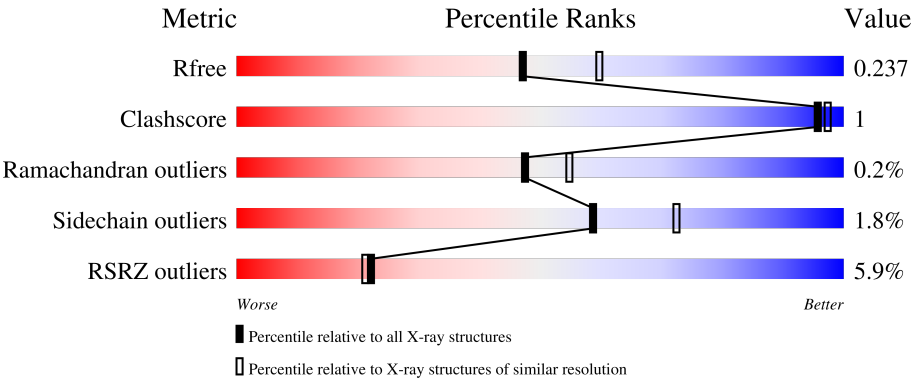
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 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 <=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	491	5% 85% · 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3526 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 Free fatty acid receptor 1,Endolysin,Free fatty acid receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3272	2120	565	574	13			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP O14842
A	-11	ASP	-	expression tag	UNP O14842
A	-10	TYR	-	expression tag	UNP O14842
A	-9	LYS	-	expression tag	UNP O14842
A	-8	ASP	-	expression tag	UNP O14842
A	-7	ASP	-	expression tag	UNP O14842
A	-6	ASP	-	expression tag	UNP O14842
A	-5	ASP	-	expression tag	UNP O14842
A	-4	LYS	-	expression tag	UNP O14842
A	-3	GLY	-	expression tag	UNP O14842
A	-2	SER	-	expression tag	UNP O14842
A	-1	ALA	-	expression tag	UNP O14842
A	0	THR	-	expression tag	UNP O14842
A	42	ALA	LEU	engineered mutation	UNP O14842
A	88	ALA	PHE	engineered mutation	UNP O14842
A	103	ALA	GLY	engineered mutation	UNP O14842
A	202	PHE	TYR	engineered mutation	UNP O14842
A	900	GLY	-	linker	UNP O14842
A	901	SER	-	linker	UNP O14842
A	1012	GLY	ARG	engineered mutation	UNP P00720
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	1137	ARG	ILE	engineered mutation	UNP P00720
A	1902	GLY	-	linker	UNP P00720
A	1903	SER	-	linker	UNP P00720
A	2301	ALA	-	expression tag	UNP O14842
A	2302	GLU	-	expression tag	UNP O14842

Continued on next page...

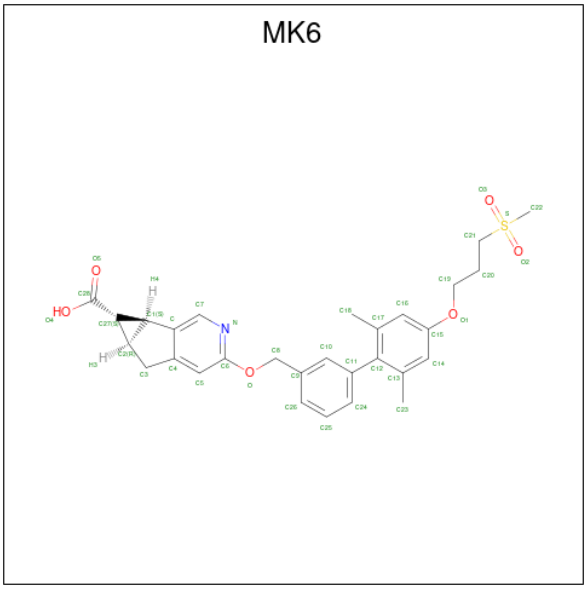
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2303	ASN	-	expression tag	UNP O14842
A	2304	LEU	-	expression tag	UNP O14842
A	2305	TYR	-	expression tag	UNP O14842
A	2306	PHE	-	expression tag	UNP O14842
A	2307	GLN	-	expression tag	UNP O14842
A	2308	GLY	-	expression tag	UNP O14842
A	2309	HIS	-	expression tag	UNP O14842
A	2310	HIS	-	expression tag	UNP O14842
A	2311	HIS	-	expression tag	UNP O14842
A	2312	HIS	-	expression tag	UNP O14842
A	2313	HIS	-	expression tag	UNP O14842
A	2314	HIS	-	expression tag	UNP O14842
A	2315	HIS	-	expression tag	UNP O14842
A	2316	HIS	-	expression tag	UNP O14842

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

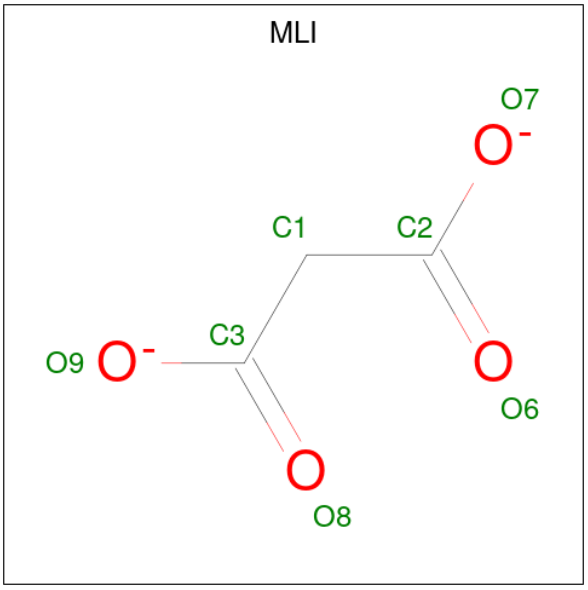
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is (5aR,6S,6aS)-3-({2',6'-dimethyl-4'-[3-(methylsulfonyl)propoxy][1,1'-biphenyl]-3-yl}methoxy)-5,5a,6,6a-tetrahydrocyclopropa[4,5]cyclopenta[1,2-c]pyridine-6-carboxylic acid (three-letter code: MK6) (formula: $C_{29}H_{31}NO_6S$).



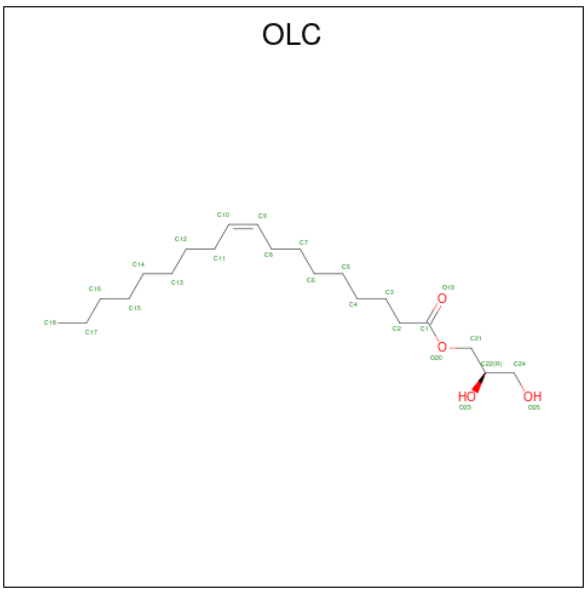
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	29	1	6	1		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



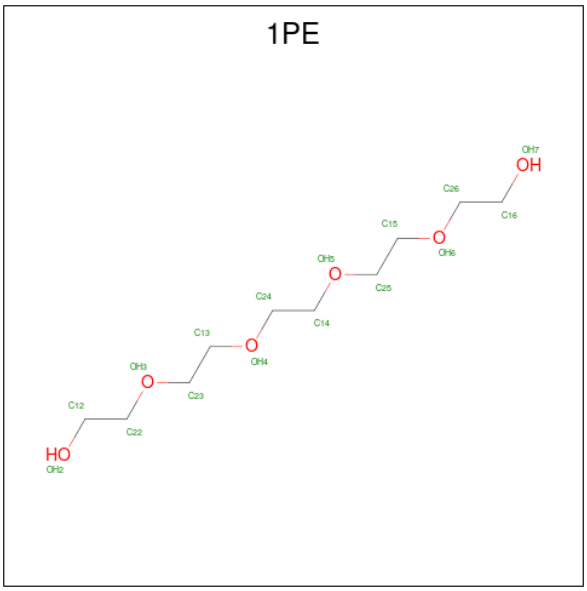
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			7	3	4			

- Molecule 5 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
5	A	1	Total C 16 16	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C O 13 11 2	0	0
5	A	1	Total C 14 14	0	0
5	A	1	Total C 9 9	0	0
5	A	1	Total C O 25 21 4	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 10 6	0	0
6	A	1	Total C O 11 7 4	0	0

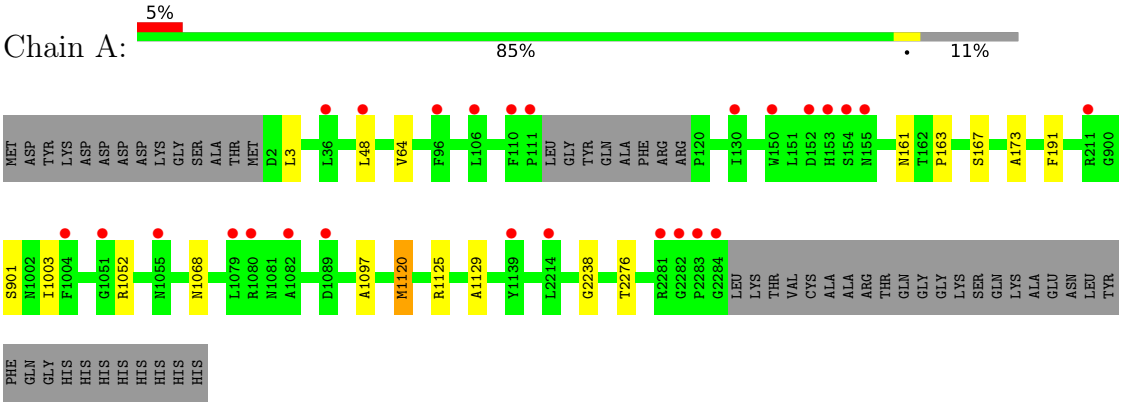
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		

3 Residue-property plots (i)

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

• Molecule 1: Free fatty acid receptor 1,Endolysin,Free fatty acid receptor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.62Å 62.60Å 106.15Å 90.00° 108.93° 90.00°	Depositor
Resolution (Å)	28.17 – 2.20 26.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.17-2.20) 95.7 (26.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.200 , 0.228 0.201 , 0.237	Depositor DCC
R_{free} test set	1177 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3526	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, OLC, MK6, 1PE, MLI

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	0.52	0/3353	0.62	0/4574

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	3272	0	3310	7	0
2	A	1	0	0	0	0
3	A	37	0	0	0	0
4	A	7	0	2	0	0
5	A	120	0	187	2	0
6	A	27	0	35	0	0
7	A	62	0	0	0	0
All	All	3526	0	3534	8	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 1.

All (8) 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:64:VAL:HG11	5:A:2411:OLC:H13	1.56	0.88
1:A:48:LEU:HD23	1:A:2276:THR:HG21	1.81	0.61
1:A:1120:MET:HG3	1:A:1125:ARG:HB2	1.87	0.56
1:A:1120:MET:HB3	1:A:1129:ALA:HB2	1.88	0.53
1:A:1003:ILE:HD13	1:A:1097:ALA:O	2.13	0.49
5:A:2407:OLC:H14A	5:A:2408:OLC:H3A	1.94	0.48
1:A:161:ASN:HB2	1:A:173:ALA:HB3	2.02	0.41
1:A:191:PHE:CZ	1:A:2238:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	433/491 (88%)	422 (98%)	10 (2%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	SER

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	330/380 (87%)	324 (98%)	6 (2%)	59 72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	163	PRO
1	A	167	SER
1	A	1052	ARG
1	A	1068	ASN
1	A	1120	MET

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	OLC	A	2407	-	8,8,24	0.34	0	7,7,25	0.76	0
5	OLC	A	2409	-	13,13,24	0.25	0	12,12,25	0.52	0
5	OLC	A	2410	-	8,8,24	0.34	0	6,7,25	0.44	0
5	OLC	A	2411	-	24,24,24	0.98	1 (4%)	25,25,25	0.83	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	1PE	A	2412	-	15,15,15	0.49	0	14,14,14	0.27	0
3	MK6	A	2402	-	41,41,41	0.38	0	52,61,61	0.85	3 (5%)
5	OLC	A	2405	-	24,24,24	0.92	1 (4%)	25,25,25	0.95	1 (4%)
5	OLC	A	2404	-	15,15,24	0.26	0	14,14,25	0.63	0
5	OLC	A	2408	-	12,12,24	2.25	2 (16%)	12,12,25	1.17	2 (16%)
5	OLC	A	2406	-	8,8,24	0.33	0	6,7,25	0.61	0
6	1PE	A	2413	-	10,10,15	0.53	0	9,9,14	0.37	0
4	MLI	A	2403	-	6,6,6	1.18	0	7,7,7	0.95	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
5	OLC	A	2407	-	-	3/6/6/24	-
5	OLC	A	2409	-	-	9/11/11/24	-
5	OLC	A	2410	-	-	3/6/6/24	-
5	OLC	A	2411	-	-	9/24/24/24	-
6	1PE	A	2412	-	-	10/13/13/13	-
3	MK6	A	2402	-	-	1/21/38/38	0/5/5/5
5	OLC	A	2405	-	-	10/24/24/24	-
5	OLC	A	2404	-	-	4/13/13/24	-
5	OLC	A	2408	-	-	4/10/10/24	-
5	OLC	A	2406	-	-	2/6/6/24	-
6	1PE	A	2413	-	-	2/8/8/13	-
4	MLI	A	2403	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2408	OLC	O19-C1	7.33	1.46	1.22
5	A	2411	OLC	O20-C1	4.57	1.46	1.33
5	A	2405	OLC	O20-C1	4.23	1.45	1.33
5	A	2408	OLC	O20-C1	-2.39	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2402	MK6	C8-O-C6	2.90	126.19	116.95
3	A	2402	MK6	O5-C28-C27	-2.63	115.78	122.78
3	A	2402	MK6	C-C1-C2	-2.21	105.26	107.46
5	A	2405	OLC	O20-C1-C2	2.13	118.61	111.91
5	A	2411	OLC	O20-C1-C2	2.11	118.54	111.91
5	A	2408	OLC	O20-C1-C2	2.08	120.71	114.03
5	A	2408	OLC	C3-C2-C1	-2.01	109.40	114.47

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2411	OLC	C21-C22-C24-O25
6	A	2412	1PE	OH7-C16-C26-OH6
5	A	2411	OLC	O20-C21-C22-O23
5	A	2411	OLC	O23-C22-C24-O25
6	A	2412	1PE	OH6-C15-C25-OH5
6	A	2412	1PE	OH5-C14-C24-OH4
5	A	2411	OLC	C5-C6-C7-C8
5	A	2409	OLC	C13-C14-C15-C16
5	A	2404	OLC	C4-C5-C6-C7
5	A	2405	OLC	C21-C22-C24-O25
5	A	2405	OLC	C14-C15-C16-C17
5	A	2411	OLC	C13-C14-C15-C16
5	A	2405	OLC	C6-C7-C8-C9
5	A	2409	OLC	C12-C13-C14-C15
5	A	2405	OLC	C2-C3-C4-C5
5	A	2407	OLC	C13-C14-C15-C16
5	A	2405	OLC	C11-C12-C13-C14
5	A	2411	OLC	C10-C11-C12-C13
5	A	2411	OLC	C11-C12-C13-C14
5	A	2411	OLC	C15-C16-C17-C18
5	A	2409	OLC	C15-C16-C17-C18
5	A	2404	OLC	C6-C7-C8-C9
5	A	2409	OLC	C10-C11-C12-C13
5	A	2404	OLC	C3-C4-C5-C6
3	A	2402	MK6	C20-C19-O1-C15
4	A	2403	MLI	C2-C1-C3-O8
5	A	2408	OLC	C6-C7-C8-C9
5	A	2409	OLC	C6-C7-C8-C9
5	A	2409	OLC	C5-C6-C7-C8
5	A	2405	OLC	C13-C14-C15-C16
5	A	2406	OLC	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	2410	OLC	C7-C8-C9-C10
5	A	2405	OLC	C15-C16-C17-C18
5	A	2410	OLC	C11-C12-C13-C14
5	A	2408	OLC	C5-C6-C7-C8
6	A	2412	1PE	C16-C26-OH6-C15
5	A	2407	OLC	C9-C10-C11-C12
6	A	2412	1PE	C13-C23-OH3-C22
6	A	2413	1PE	C15-C25-OH5-C14
6	A	2412	1PE	C14-C24-OH4-C13
6	A	2412	1PE	C24-C14-OH5-C25
6	A	2412	1PE	C12-C22-OH3-C23
4	A	2403	MLI	C2-C1-C3-O9
5	A	2410	OLC	C10-C11-C12-C13
5	A	2407	OLC	C11-C12-C13-C14
6	A	2412	1PE	OH2-C12-C22-OH3
5	A	2404	OLC	C5-C6-C7-C8
4	A	2403	MLI	C3-C1-C2-O6
6	A	2412	1PE	OH4-C13-C23-OH3
5	A	2405	OLC	O23-C22-C24-O25
5	A	2409	OLC	C11-C12-C13-C14
6	A	2413	1PE	OH6-C15-C25-OH5
5	A	2409	OLC	C9-C10-C11-C12
5	A	2408	OLC	C2-C3-C4-C5
5	A	2406	OLC	C9-C10-C11-C12
5	A	2411	OLC	O20-C21-C22-C24
4	A	2403	MLI	C3-C1-C2-O7
5	A	2408	OLC	C7-C8-C9-C10
5	A	2409	OLC	C7-C8-C9-C10
5	A	2405	OLC	C7-C8-C9-C10
5	A	2405	OLC	O20-C21-C22-O23

There are no ring outliers.

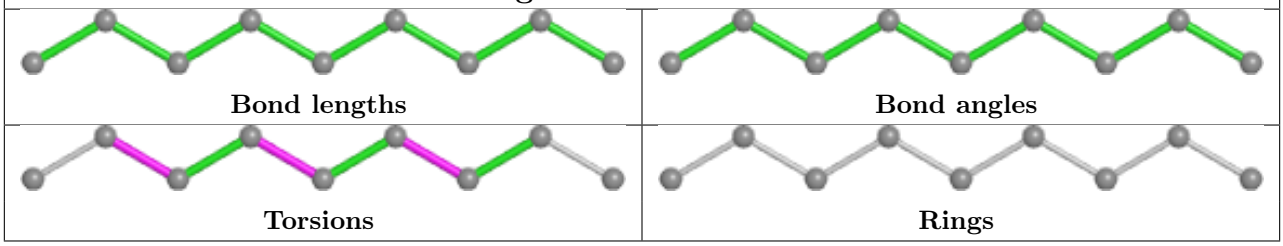
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2407	OLC	1	0
5	A	2411	OLC	1	0
5	A	2408	OLC	1	0

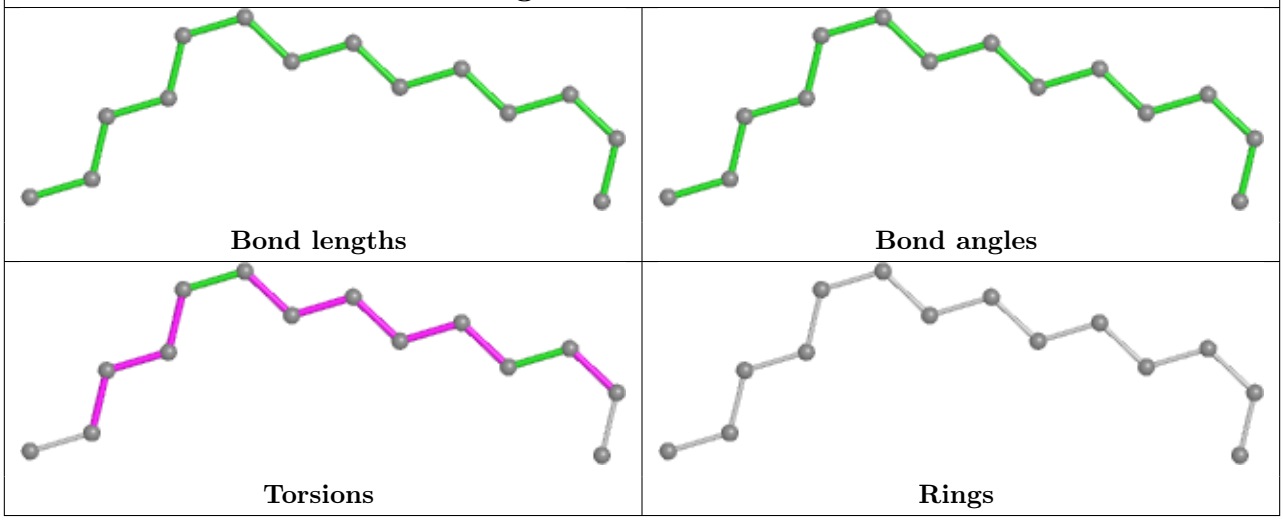
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

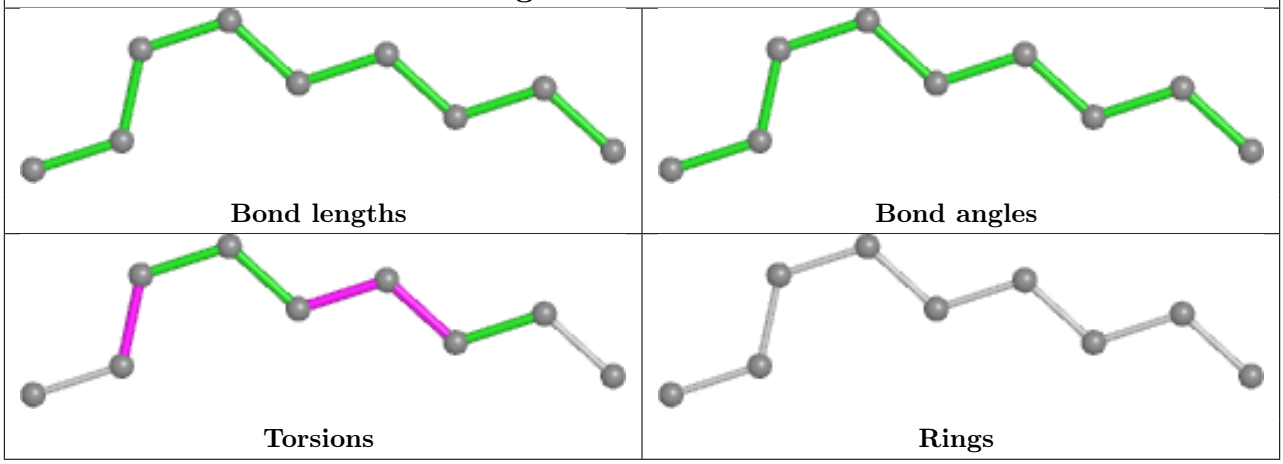
Ligand OLC A 2407



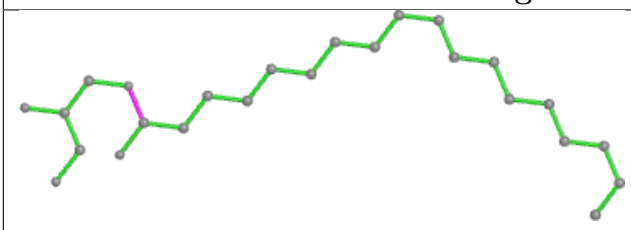
Ligand OLC A 2409



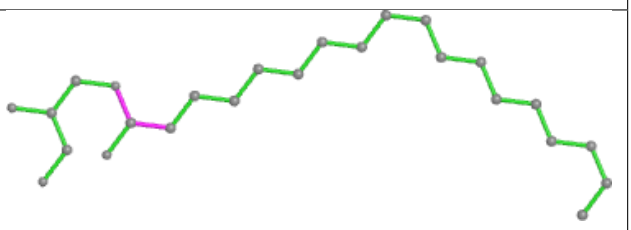
Ligand OLC A 2410



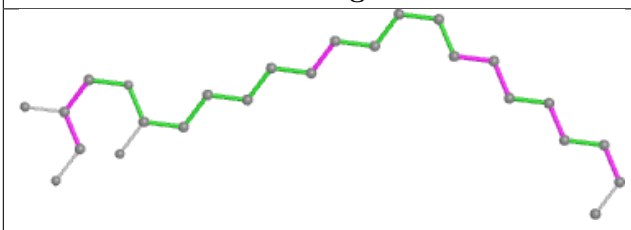
Ligand OLC A 2411



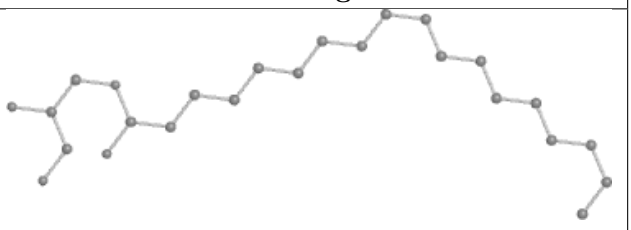
Bond lengths



Bond angles

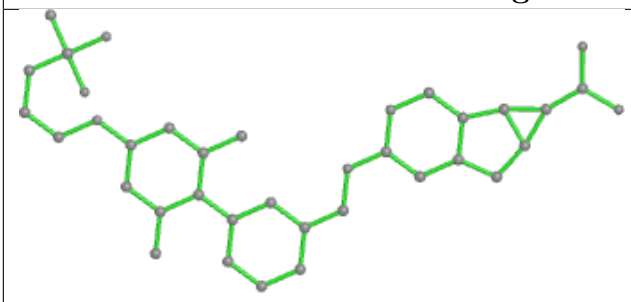


Torsions

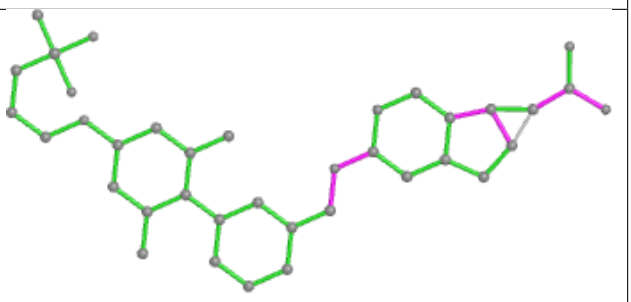


Rings

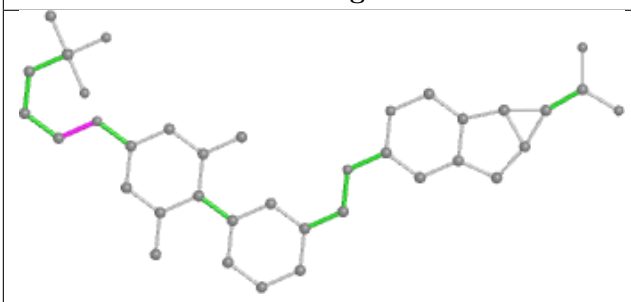
Ligand MK6 A 2402



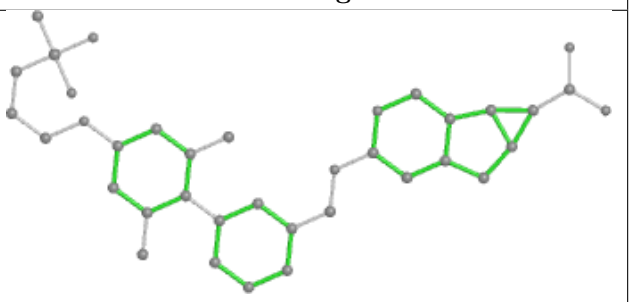
Bond lengths



Bond angles

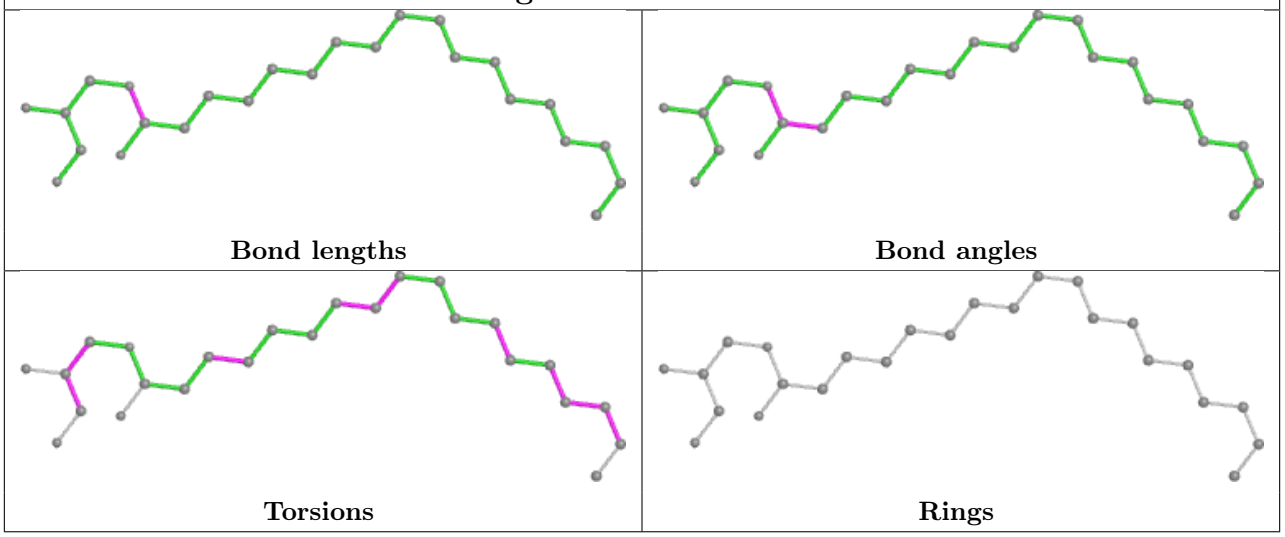


Torsions

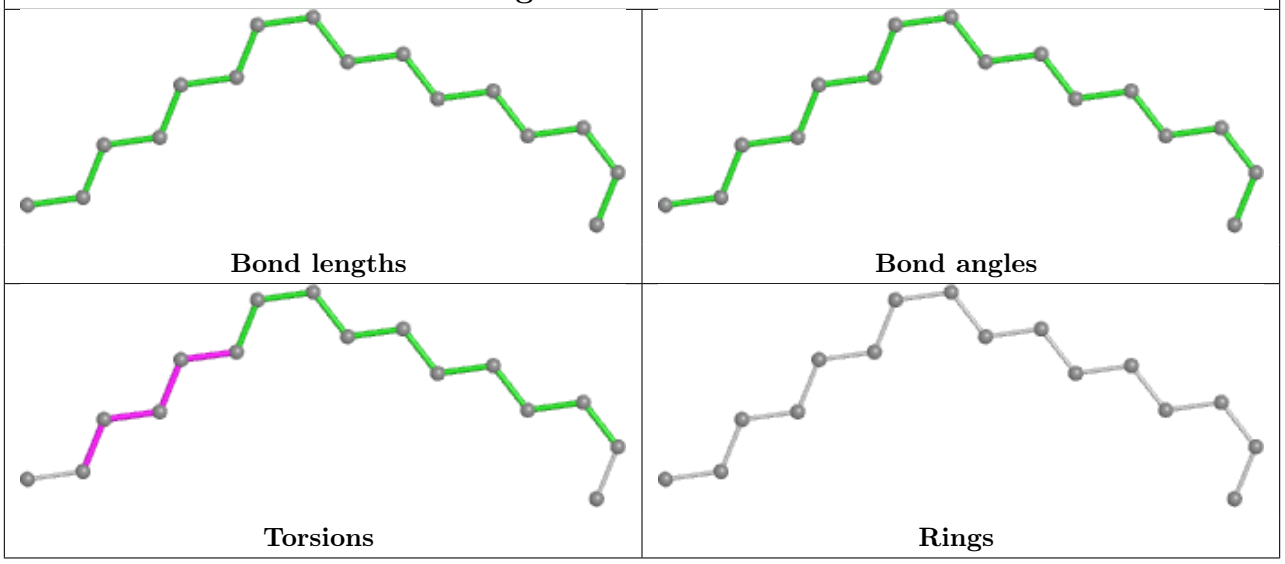


Rings

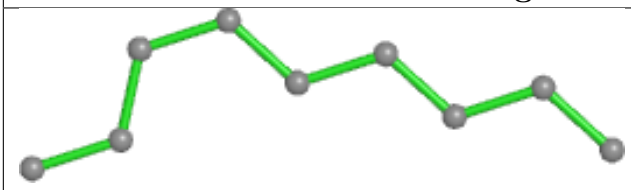
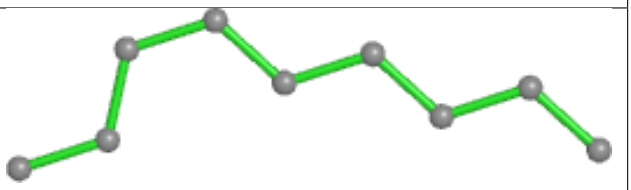
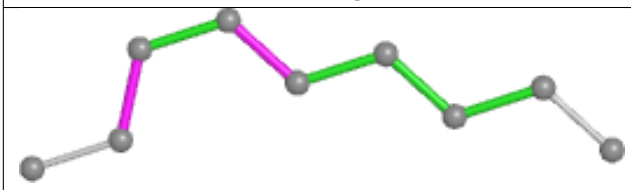
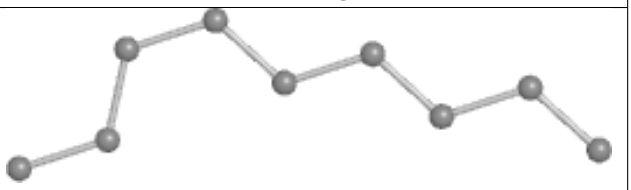
Ligand OLC A 2405



Ligand OLC A 2404



Ligand OLC A 2408

Ligand OLC A 2406	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	437/491 (89%)	0.19	26 (5%)	22	21	35, 50, 82, 99	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	HIS	8.2
1	A	155	ASN	5.8
1	A	36	LEU	5.7
1	A	2284	GLY	5.0
1	A	150	TRP	4.4
1	A	2283	PRO	3.9
1	A	2282	GLY	3.8
1	A	110	PHE	3.6
1	A	111	PRO	3.6
1	A	152	ASP	3.4
1	A	2281	ARG	3.3
1	A	211	ARG	3.3
1	A	154	SER	3.1
1	A	2214	LEU	2.9
1	A	130	ILE	2.6
1	A	1004	PHE	2.5
1	A	1079	LEU	2.5
1	A	1082	ALA	2.4
1	A	1080	ARG	2.4
1	A	1051	GLY	2.4
1	A	48	LEU	2.3
1	A	96	PHE	2.2
1	A	106	LEU	2.2
1	A	1089	ASP	2.2
1	A	1055	ASN	2.1
1	A	1139	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

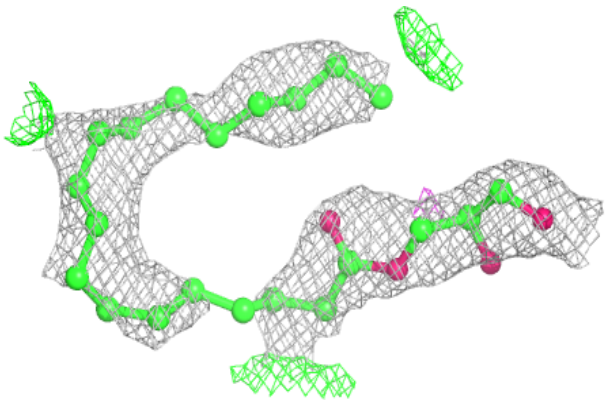
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

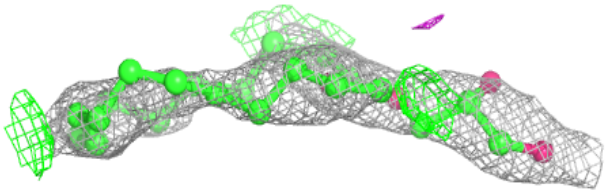
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLC	A	2411	25/25	0.73	0.29	81,84,88,91	0
6	1PE	A	2412	16/16	0.73	0.30	82,84,94,95	0
4	MLI	A	2403	7/7	0.77	0.31	74,78,79,80	0
5	OLC	A	2408	13/25	0.80	0.28	62,66,82,83	0
5	OLC	A	2409	14/25	0.81	0.24	68,73,78,78	0
5	OLC	A	2410	9/25	0.82	0.16	61,65,71,71	0
5	OLC	A	2405	25/25	0.83	0.28	52,58,81,83	0
3	MK6	A	2402	37/37	0.85	0.14	35,41,92,93	0
6	1PE	A	2413	11/16	0.87	0.27	68,75,84,85	0
5	OLC	A	2406	9/25	0.90	0.14	57,59,62,62	0
5	OLC	A	2404	16/25	0.92	0.12	52,59,64,65	0
5	OLC	A	2407	9/25	0.92	0.15	63,64,75,78	0
2	NA	A	2401	1/1	1.00	0.18	36,36,36,36	0

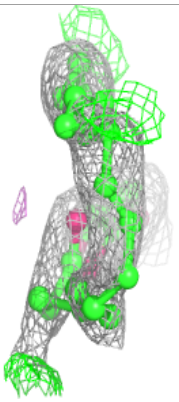
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 2411:

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

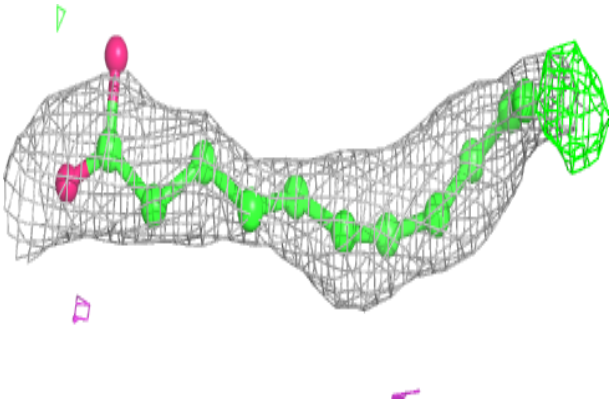


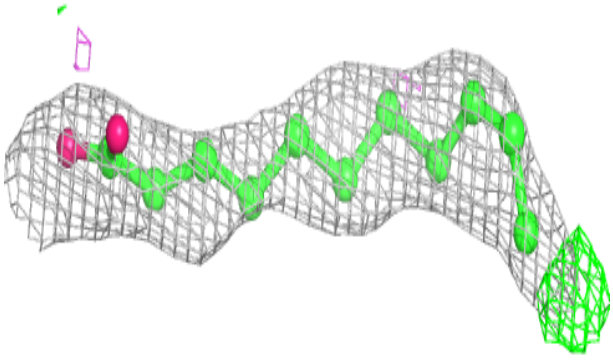


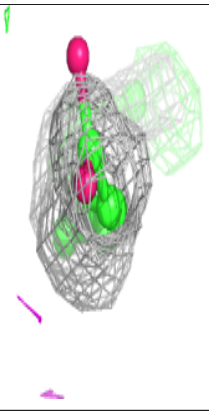


Electron density around OLC A 2408:

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

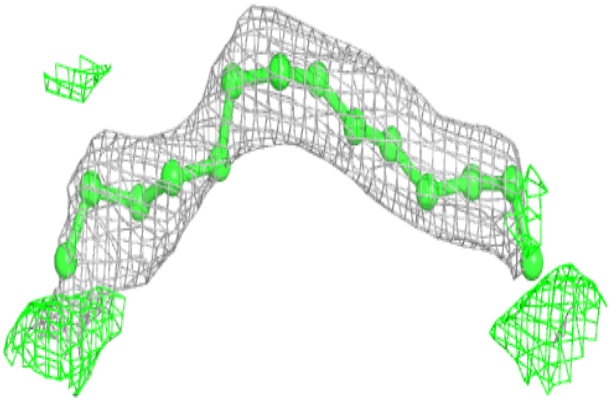


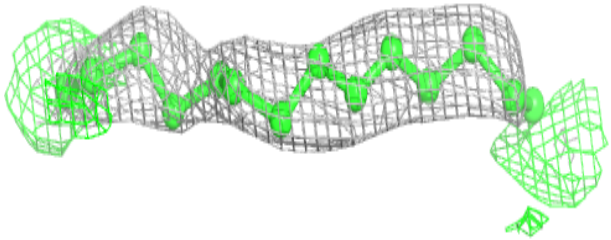


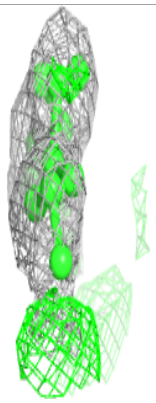


Electron density around OLC A 2409:

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

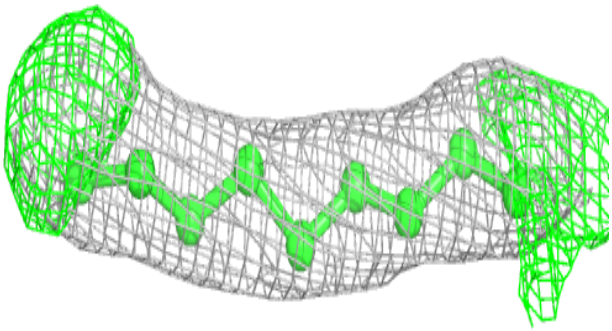


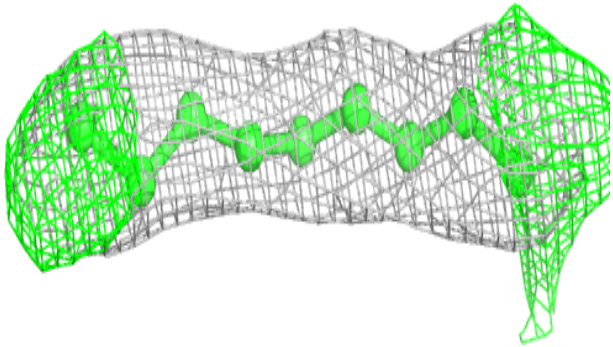


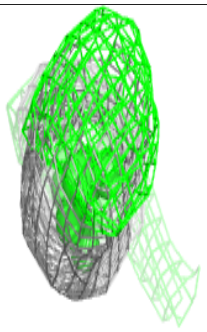


Electron density around OLC A 2410:

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

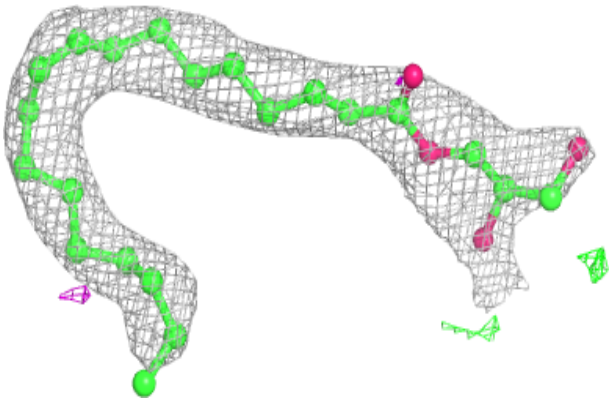


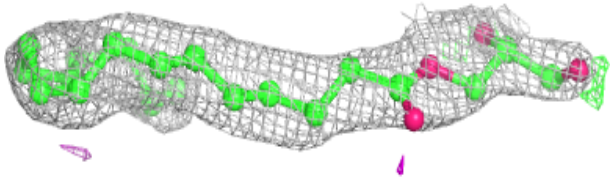


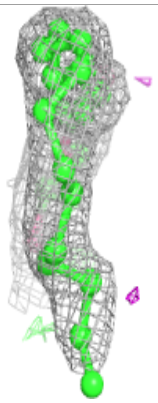


Electron density around OLC A 2405:

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

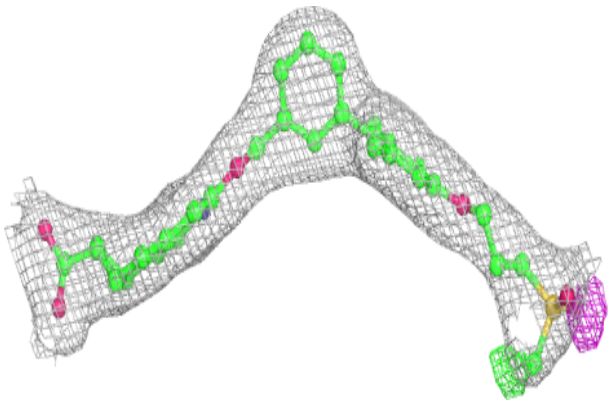


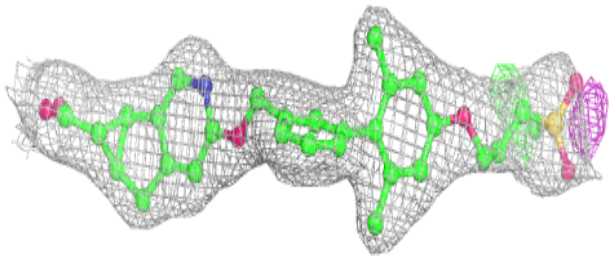


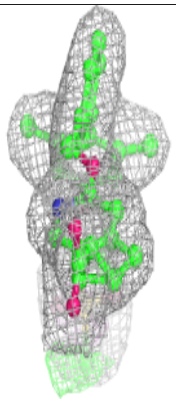


Electron density around MK6 A 2402:

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

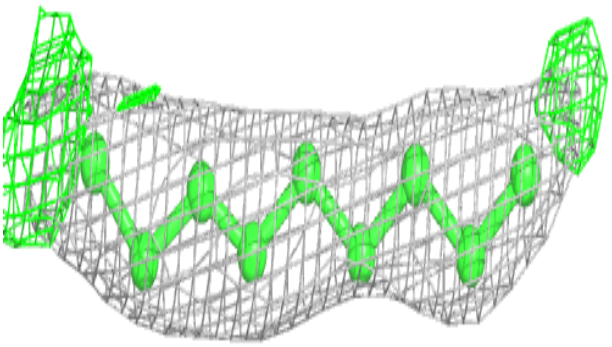


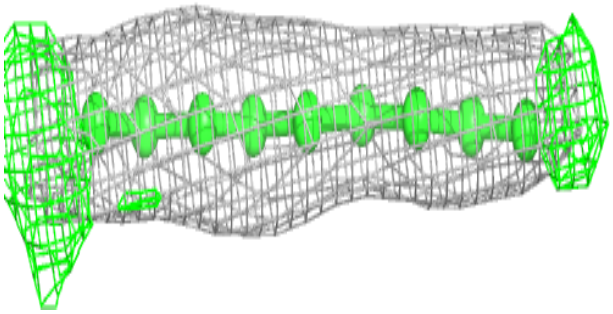


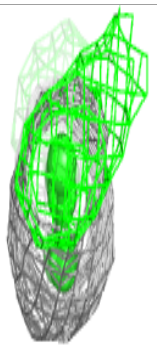


Electron density around OLC A 2406:

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

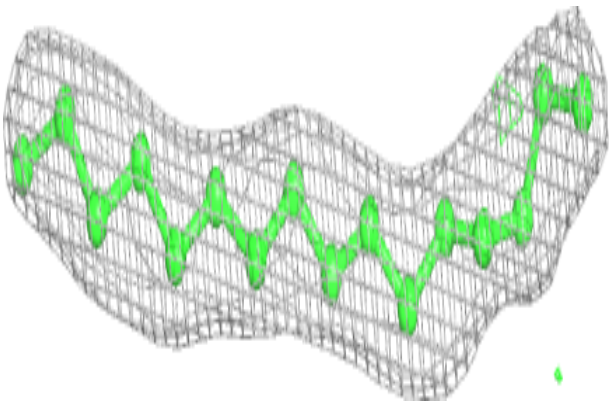


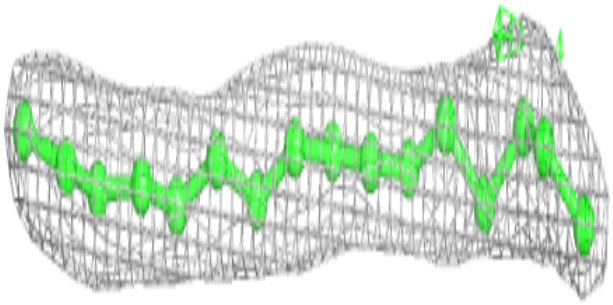


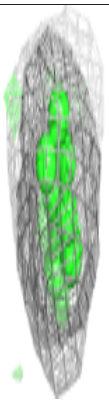


Electron density around OLC A 2404:

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

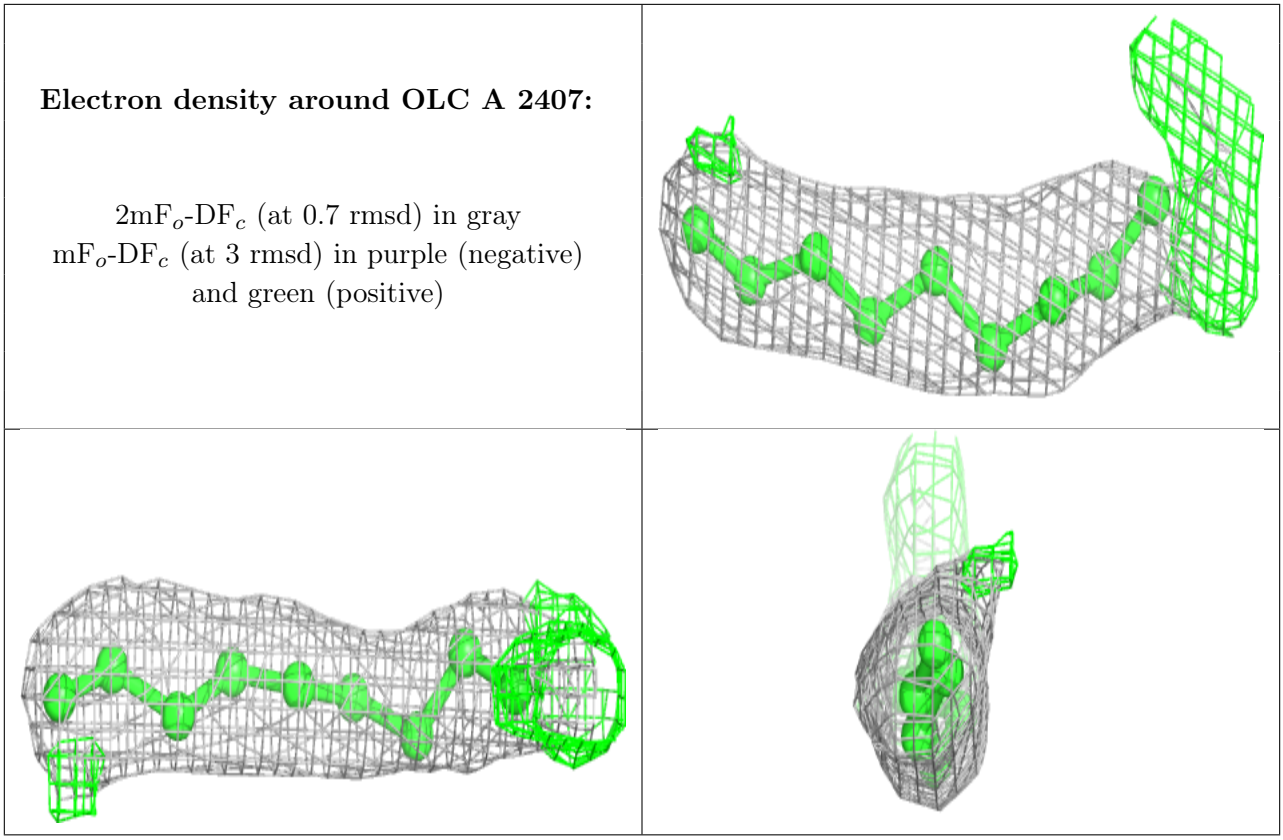






Electron density around OLC A 2407:

$2mF_o$-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.