wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 11:09 PM EDT

PDB ID	:	6CXH
Title	:	Crystal structure of particulate methane monooxygenase from Methylomicrobium alcaliphilum 20Z
Authors	:	Ro, S.Y.; Rosenzweig, A.C.
Deposited on	:	2018-04-03
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

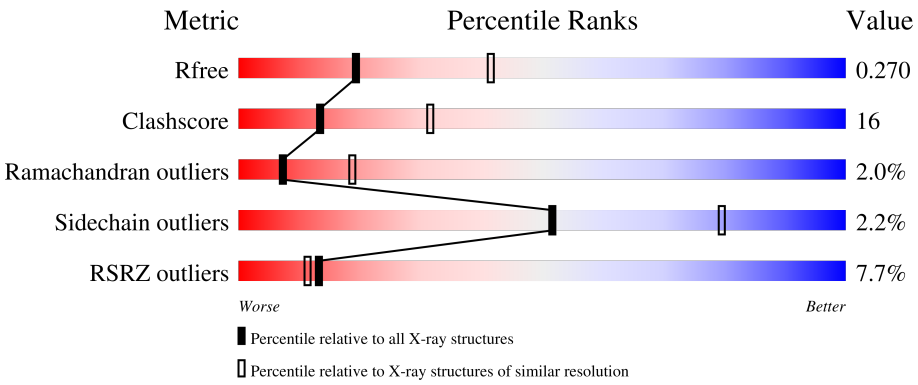
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	414	10%, 63%, 28%, 8%
2	B	247	2%, 61%, 36%
3	C	250	3%, 26%, 12%, 60%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5807 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 Particulate methane monooxygenase, B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2970	1906	495	554	15	0	0	0

- Molecule 2 is a protein called Particulate methane monooxygenase, A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	241	1968	1326	313	319	10	0	0	0

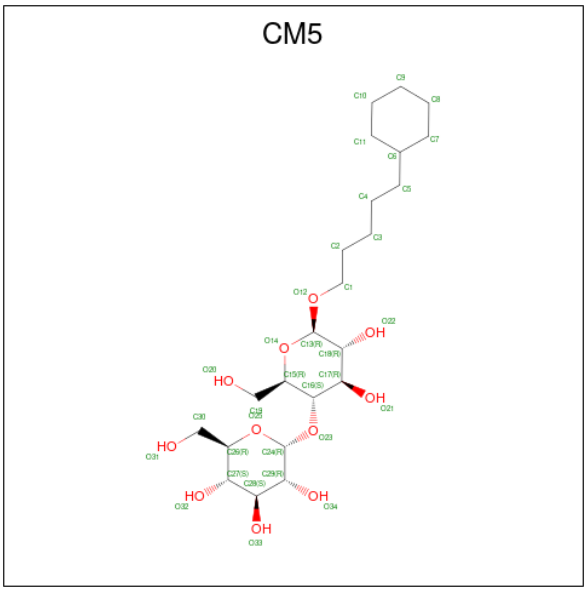
- Molecule 3 is a protein called Particulate methane monooxygenase, C subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	101	800	537	129	130	4	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
4	A	1	1	1	0	0

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



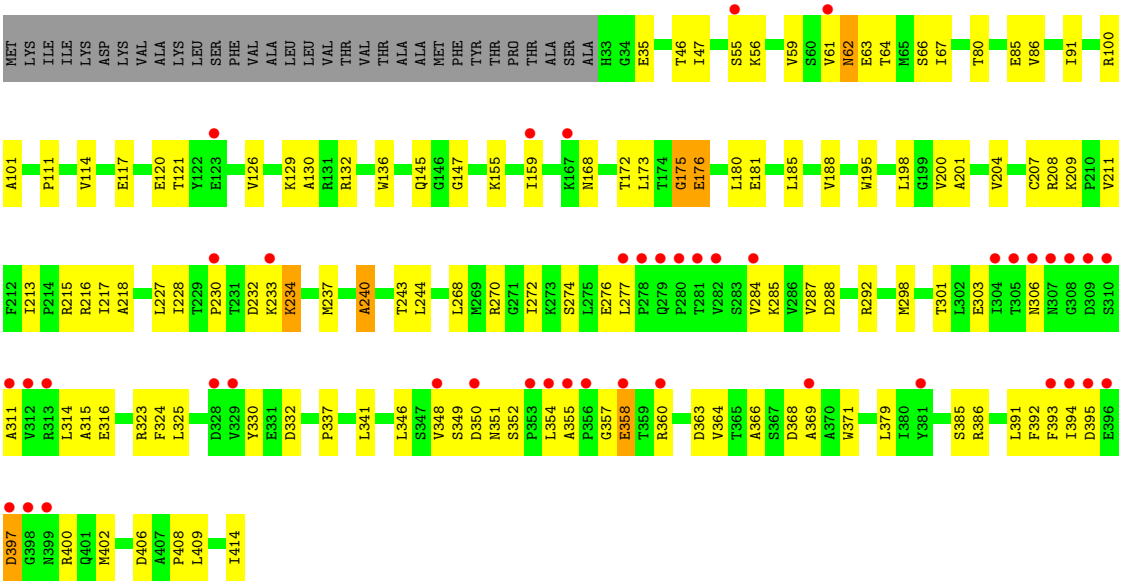
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	34	23	11	0	0
			Total	C	O		
5	C	1	34	23	11	0	0

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.

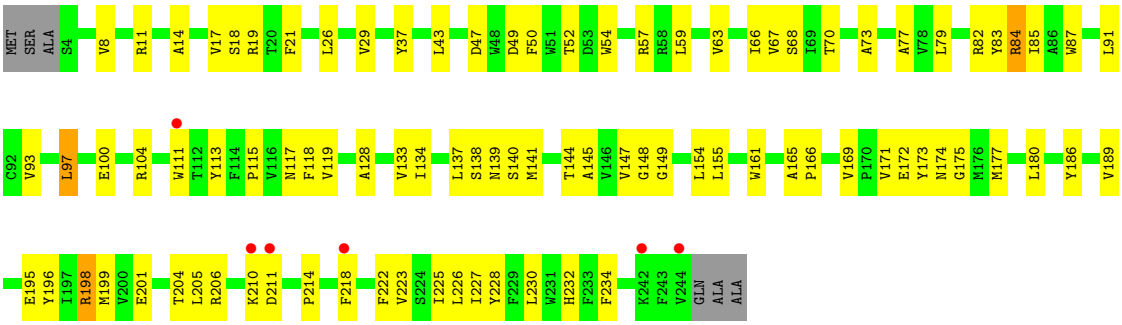
• Molecule 1: Particulate methane monooxygenase, B subunit

Chain A: 10% 63% 28% • 8%



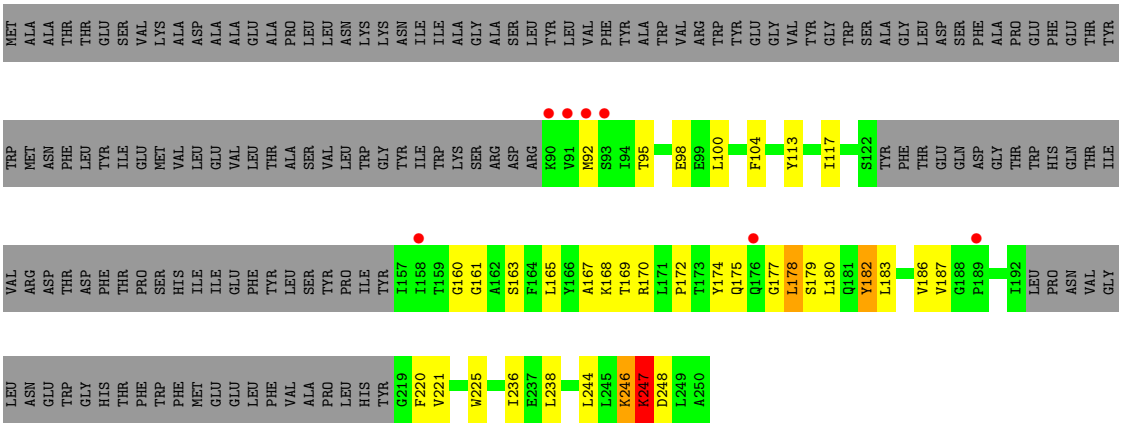
• Molecule 2: Particulate methane monooxygenase, A subunit

Chain B: 2% 61% 36% • •



• Molecule 3: Particulate methane monooxygenase, C subunit

Chain C: 3% 26% 12% • 60%


MET ALA ALA THR THR GLU SER VAL LYS ALA ASP ALA ALA GLU ALA PRO LEU LEU ASN LYS LYS ASN ILE ILE ALA GLY ALA SER LEU TYR LEU VAL PHE TYR ALA TRP VAL ARG TRP TYR GLU GLY VAL TYR GLY TRP SER ALA GLY LEU ASP SER PHE ALA PRO GLU PHE GLU THR TYR
TRP MET ASN PHE LEU TYR ILE GLU MET VAL LEU GLU VAL LEU THR ALA SER VAL LEU TRP GLY TYR ILE TRP LYS SER ARG ASP ARG K90 V91 M92 S93 I94 T95 E98 E99 L100 F104 Y113 I117 S122 TYR PHE THR GLU GLN ASP GLY THR TRP HIS GLN THR ILE
VAL ARG ASP THR ASP PHE THR PRO SER HIS ILE ILE GLU PHE TYR LEU SER TYR PRO ILE TYR I157 I158 T159 G160 G161 A162 S163 F164 L165 Y166 A167 K168 T169 R170 L171 P172 T173 Y174 Q175 Q176 G177 L178 S179 L180 Q181 Y182 L183 V186 V187 G188 P189 I192 LEU PRO ASN VAL GLY
LEU ASN GLU TRP GLY HIS THR PHE TRP PHE MET GLU GLU LEU PHE VAL ALA PRO LEU HIS TYR G219 F220 V221 W225 I236 E237 L238 L244 L245 K246 K247 D248 L249 A250

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	143.84Å 143.84Å 146.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.58 – 2.70 39.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.58-2.70) 99.1 (39.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.213 , 0.268 0.228 , 0.270	Depositor DCC
R_{free} test set	2359 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CM5, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/3048	0.68	0/4155
2	B	0.52	0/2044	0.71	1/2796 (0.0%)
3	C	0.45	0/820	0.69	1/1107 (0.1%)
All	All	0.50	0/5912	0.69	2/8058 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	97	LEU	CA-CB-CG	-10.29	91.62	115.30
3	C	247	LYS	C-N-CA	6.52	138.00	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	LYS	Peptide
1	A	276	GLU	Peptide
3	C	246	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	247	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2921	100	0
2	B	1968	0	1930	74	0
3	C	800	0	829	32	0
4	A	1	0	0	0	0
5	A	34	0	42	2	0
5	C	34	0	42	1	0
All	All	5807	0	5764	186	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 16.

The worst 5 of 186 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:100:ARG:NH2	2:B:186:TYR:O	2.08	0.86
1:A:316:GLU:OE2	1:A:323:ARG:HD2	1.75	0.85
1:A:323:ARG:NH1	1:A:332:ASP:OD1	2.16	0.79
1:A:46:THR:HG23	1:A:47:ILE:H	1.47	0.79
1:A:173:LEU:HD21	2:B:172:GLU:HB2	1.68	0.76

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	380/414 (92%)	335 (88%)	37 (10%)	8 (2%)	7 18
2	B	239/247 (97%)	213 (89%)	23 (10%)	3 (1%)	12 30
3	C	95/250 (38%)	77 (81%)	15 (16%)	3 (3%)	4 9
All	All	714/911 (78%)	625 (88%)	75 (10%)	14 (2%)	7 19

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLY
1	A	176	GLU
2	B	70	THR
2	B	174	ASN
3	C	187	VAL

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	317/343 (92%)	312 (98%)	5 (2%)	62 85
2	B	204/207 (99%)	198 (97%)	6 (3%)	42 71
3	C	83/211 (39%)	81 (98%)	2 (2%)	49 77
All	All	604/761 (79%)	591 (98%)	13 (2%)	52 79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	141	MET
2	B	177	MET
3	C	220	PHE
2	B	234	PHE
3	C	182	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	232	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	CM5	C	301	-	36,36,36	1.20	4 (11%)	49,49,49	1.21	5 (10%)
5	CM5	A	502	-	36,36,36	1.24	4 (11%)	49,49,49	1.51	9 (18%)

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	CM5	C	301	-	-	6/17/65/65	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CM5	A	502	-	-	8/17/65/65	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	CM5	O14-C13	3.80	1.51	1.41
5	C	301	CM5	O14-C13	3.70	1.51	1.41
5	C	301	CM5	O25-C24	2.91	1.49	1.41
5	A	502	CM5	O25-C24	2.79	1.49	1.41
5	A	502	CM5	O25-C26	2.45	1.50	1.44

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	502	CM5	O25-C26-C27	4.62	118.08	109.69
5	A	502	CM5	C10-C11-C6	-3.65	105.26	112.15
5	A	502	CM5	C9-C8-C7	2.97	117.46	111.42
5	C	301	CM5	O14-C15-C16	2.96	115.98	109.75
5	A	502	CM5	C8-C7-C6	-2.78	106.89	112.15

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	CM5	C27-C26-C30-O31
5	C	301	CM5	O25-C24-O23-C16
5	C	301	CM5	O25-C26-C30-O31
5	A	502	CM5	O14-C15-C19-O20
5	A	502	CM5	C16-C15-C19-O20

There are no ring outliers.

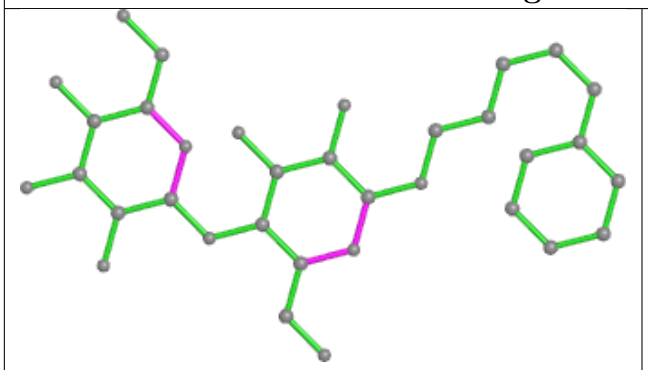
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	CM5	1	0
5	A	502	CM5	2	0

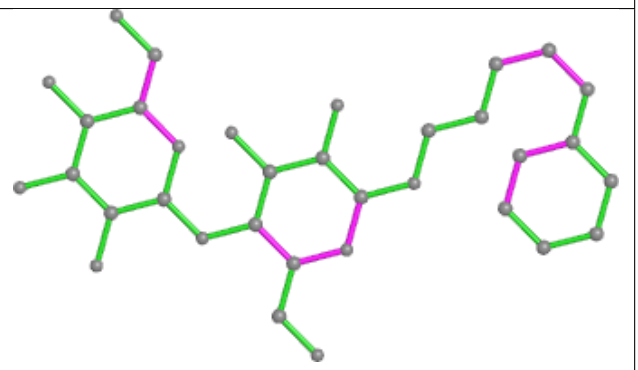
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

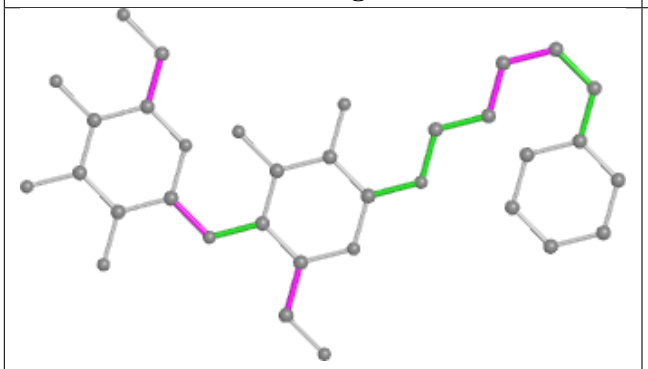
Ligand CM5 C 301



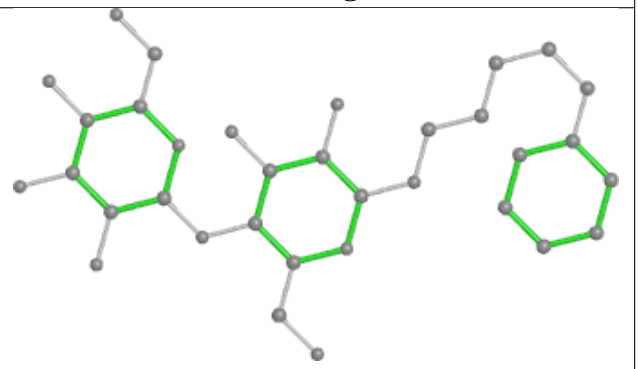
Bond lengths



Bond angles

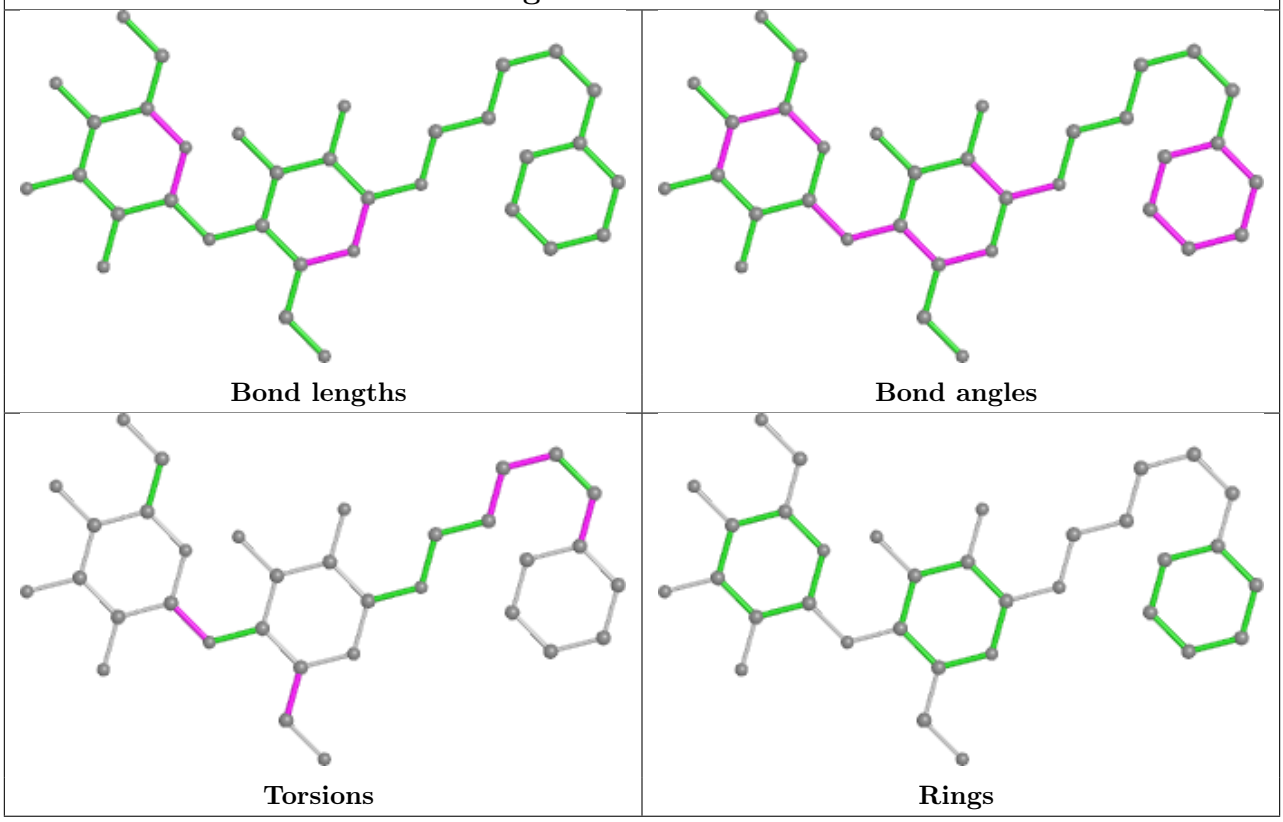


Torsions



Rings

Ligand CM5 A 502



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	382/414 (92%)	0.29	43 (11%)	5	4	10, 35, 71, 114	0
2	B	241/247 (97%)	0.20	6 (2%)	57	59	10, 25, 52, 122	0
3	C	101/250 (40%)	0.31	7 (6%)	16	15	14, 45, 76, 97	0
All	All	724/911 (79%)	0.26	56 (7%)	13	11	10, 32, 70, 122	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	PRO	7.1
1	A	281	THR	5.4
1	A	313	ARG	5.4
3	C	158	ILE	5.0
1	A	312	VAL	5.0

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)

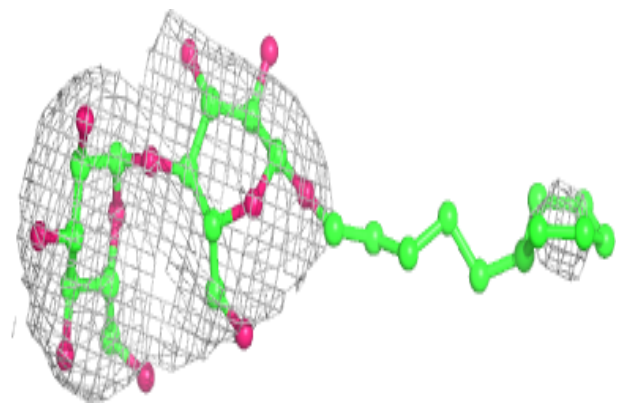
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

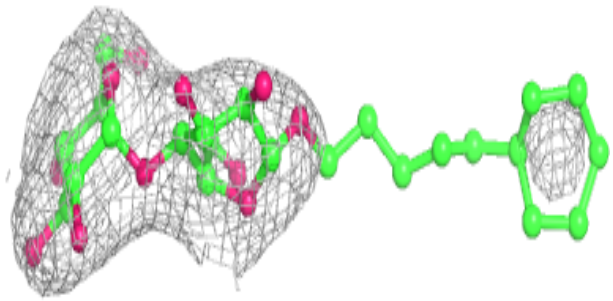
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CM5	C	301	34/34	0.79	0.35	47,81,99,101	0
5	CM5	A	502	34/34	0.81	0.19	29,78,117,122	0
4	CU	A	501	1/1	0.98	0.16	45,45,45,45	0

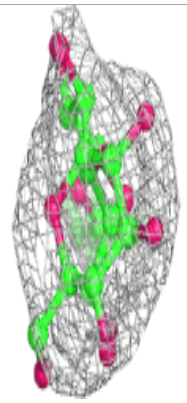
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CM5 C 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

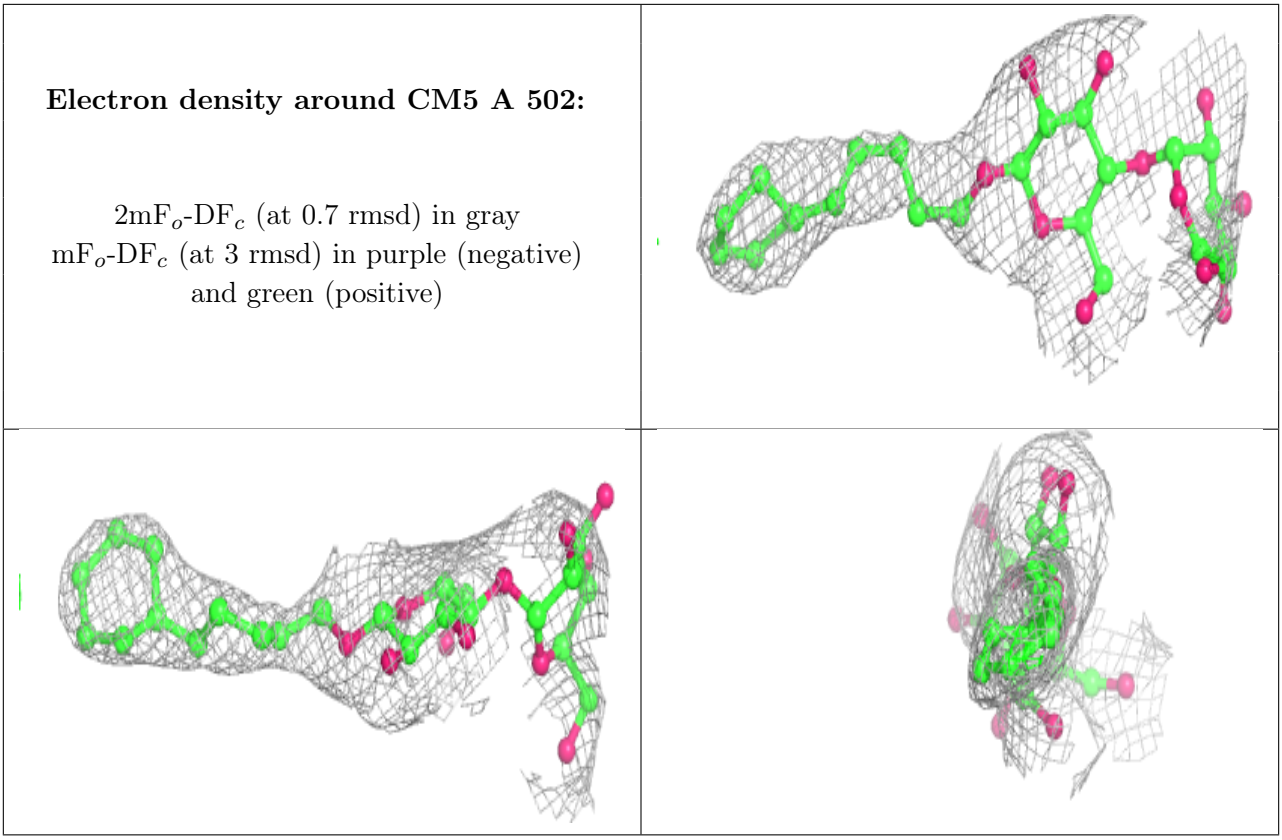






Electron density around CM5 A 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.