wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 03:33 pm BST

PDB ID	:	4PHZ
Title	:	Crystal structure of particulate methane monooxygenase from Methylocystis sp. ATCC 49242 (Rockwell)
Authors	:	Sirajuddin, S.; Rosenzweig, A.C.
Deposited on	:	2014-05-07
Resolution	:	2.59 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 following versions of software and data (see references (i)) were used in the production of this report:

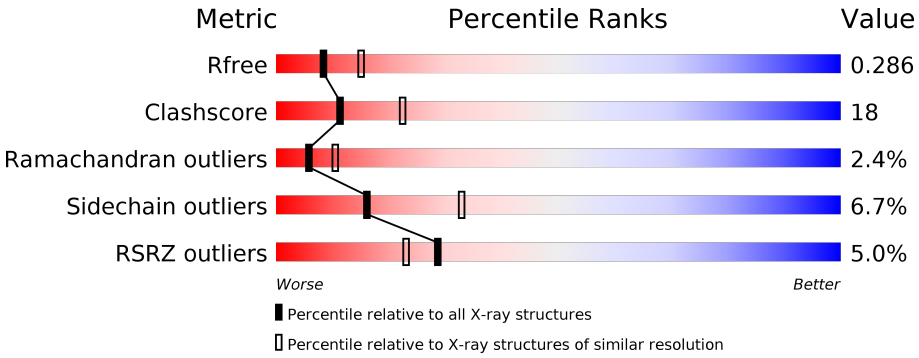
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	D	24	79% 21%
1	H	24	79% . 17%
1	N	24	79% 21%
2	C	256	6% 53% 27% . 16%
2	G	256	7% 53% 27% . 17%
2	K	256	5% 50% 29% . 17%

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Mol	Chain	Length	Quality of chain
3	A	420	6% 62% 26% 8%
3	E	420	2% 61% 26% 8%
3	I	420	8% 66% 22% 8%
4	B	252	4% 63% 29%
4	F	252	% 66% 26%
4	J	252	% 65% 26% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PGT	K	302	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20853 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 unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	19	Total	C	N	O	0	0	0
			95	57	19	19			
1	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
1	N	24	Total	C	N	O	0	0	0
			120	72	24	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	213	Total	C	N	O	S	0	0	0
			1738	1166	275	289	8			
2	C	214	Total	C	N	O	S	0	0	0
			1742	1168	276	290	8			
2	G	212	Total	C	N	O	S	0	0	0
			1731	1161	274	288	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			
3	E	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			
3	I	388	Total	C	N	O	S	0	0	0
			3026	1946	521	555	4			

- Molecule 4 is a protein called Particulate methane monooxygenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

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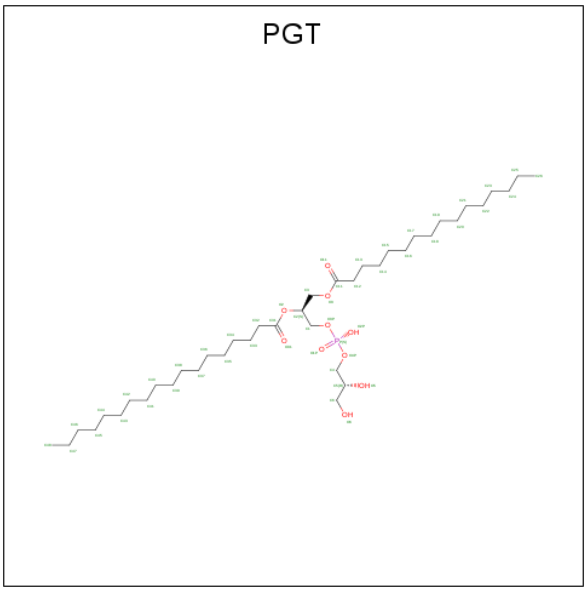
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
4	J	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cu	0	0
			1	1		
5	K	1	Total	Cu	0	0
			1	1		
5	E	1	Total	Cu	0	0
			1	1		
5	I	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	A	1	Total	Cu	0	0
			1	1		

- Molecule 6 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	O	P	0	0
			51	40	10	1		
6	C	1	Total	C	O	P	0	0
			51	40	10	1		
6	G	1	Total	C	O	P	0	0
			51	40	10	1		
6	G	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 7 is water.

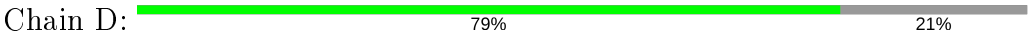
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	7	Total	O	0	0
			7	7		
7	A	13	Total	O	0	0
			13	13		
7	B	11	Total	O	0	0
			11	11		
7	E	25	Total	O	0	0
			25	25		
7	I	12	Total	O	0	0
			12	12		
7	F	18	Total	O	0	0
			18	18		
7	J	16	Total	O	0	0
			16	16		
7	C	4	Total	O	0	0
			4	4		
7	G	11	Total	O	0	0
			11	11		

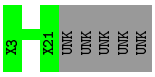
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: unknown peptide

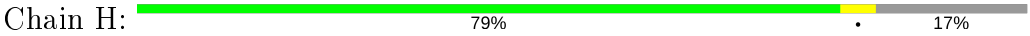
Chain D:

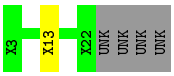




- Molecule 1: unknown peptide

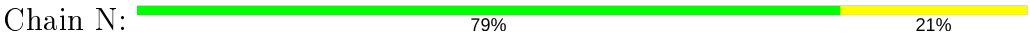
Chain H:





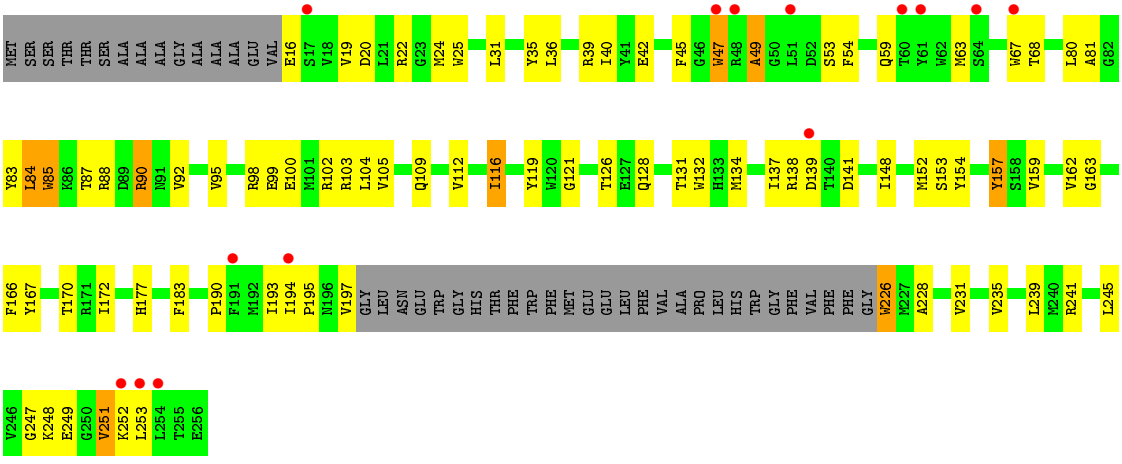
- Molecule 1: unknown peptide

Chain N:



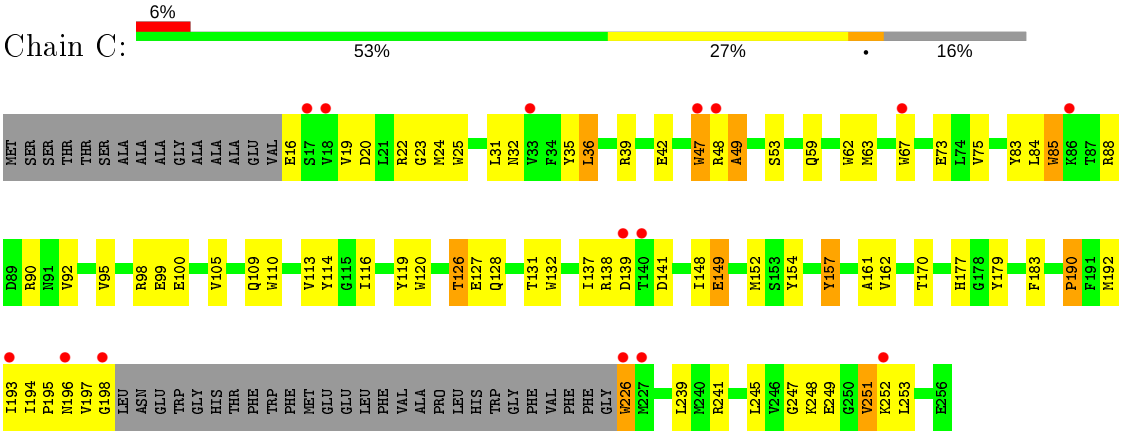
- Molecule 2: Particulate methane monooxygenase subunit C

Chain K:



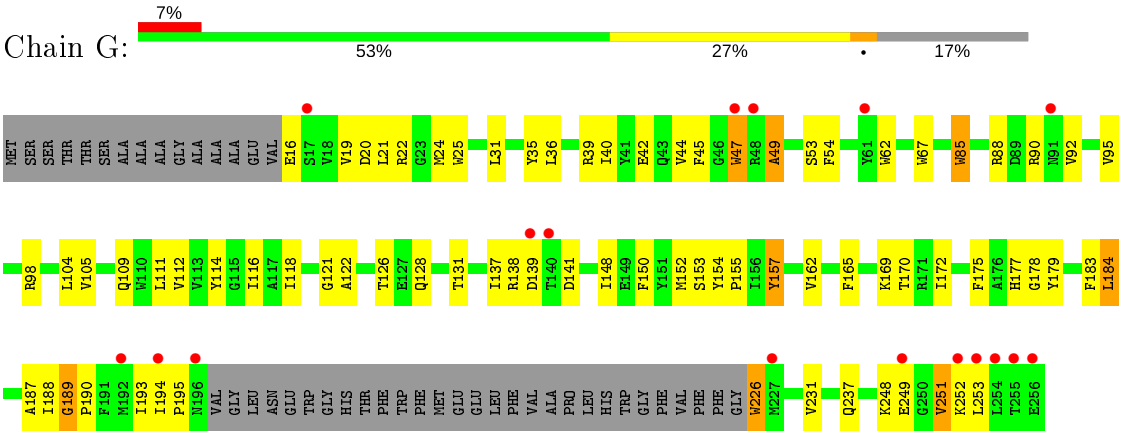
• Molecule 2: Particulate methane monooxygenase subunit C

Chain C:



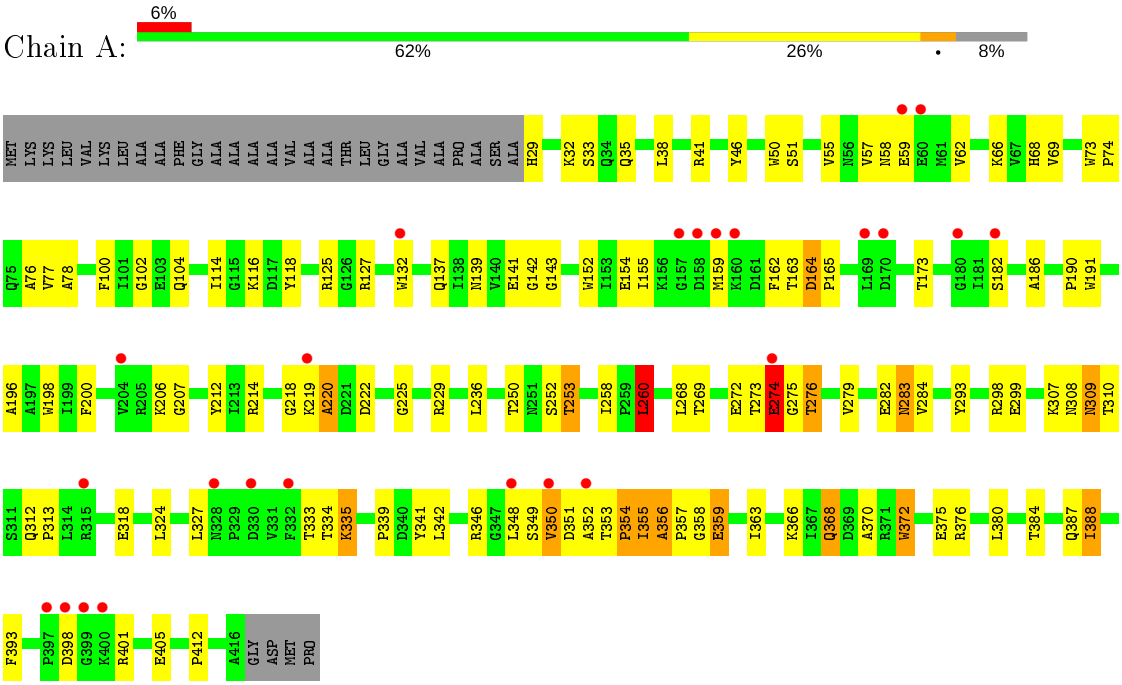
• Molecule 2: Particulate methane monooxygenase subunit C

Chain G:



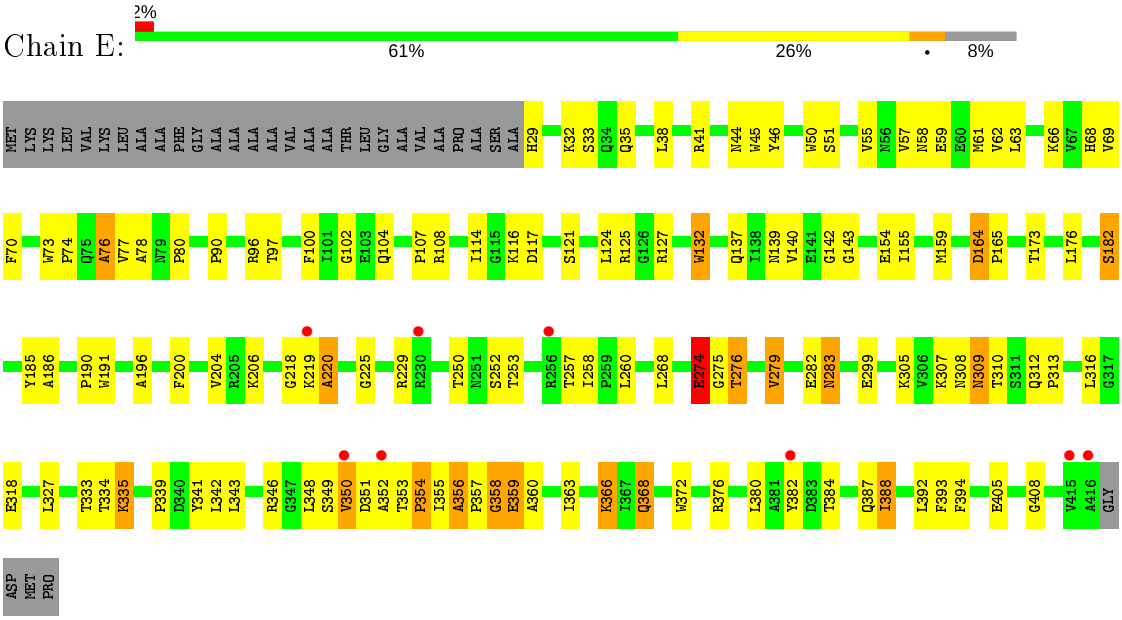
• Molecule 3: Particulate methane monooxygenase subunit B

Chain A:



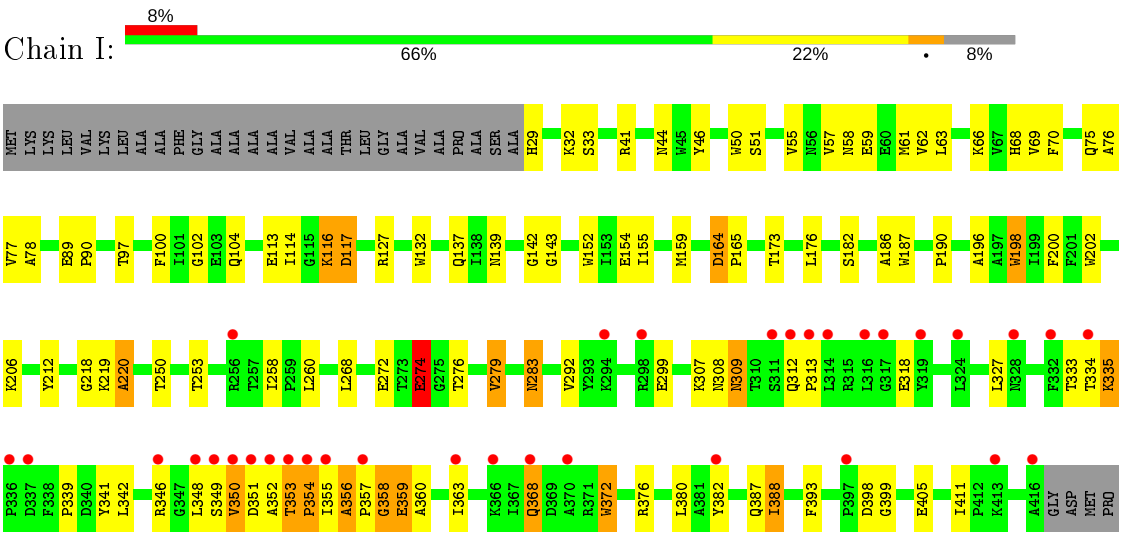
• Molecule 3: Particulate methane monooxygenase subunit B

Chain E:



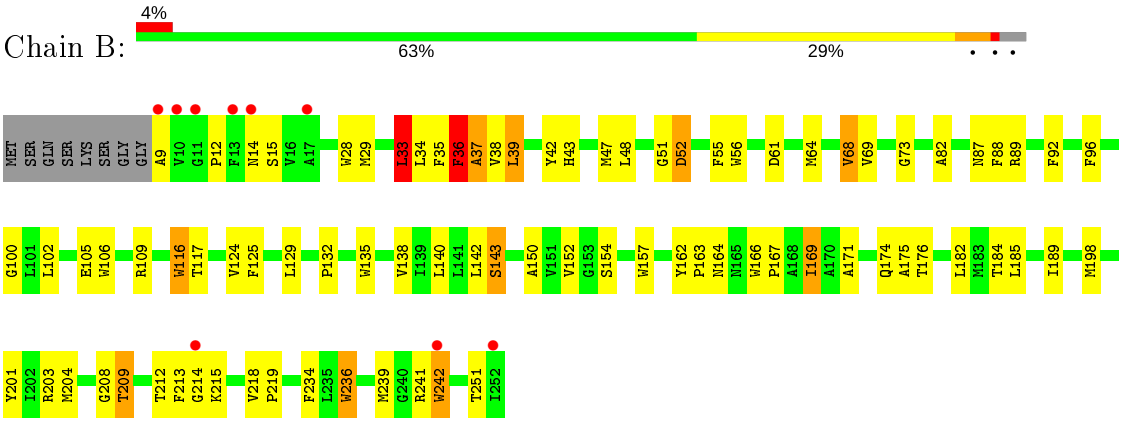
• Molecule 3: Particulate methane monooxygenase subunit B

Chain I:



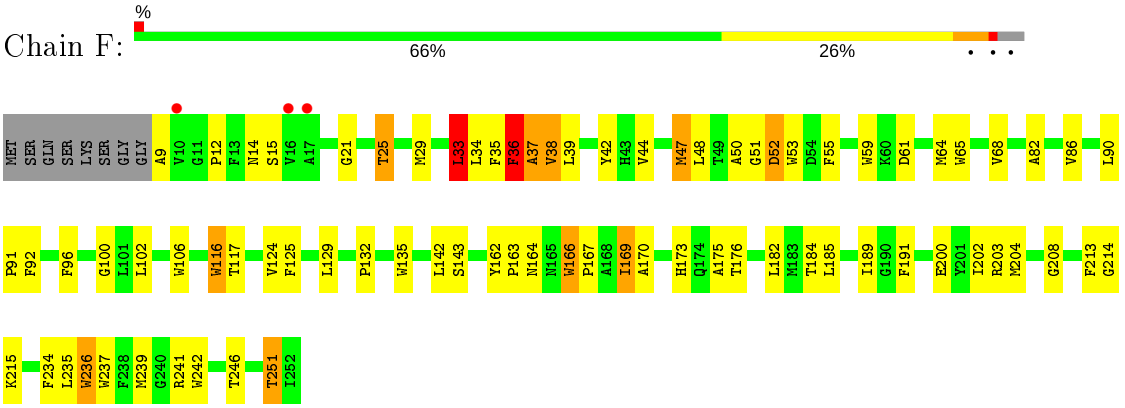
• Molecule 4: Particulate methane monooxygenase subunit A

Chain B:



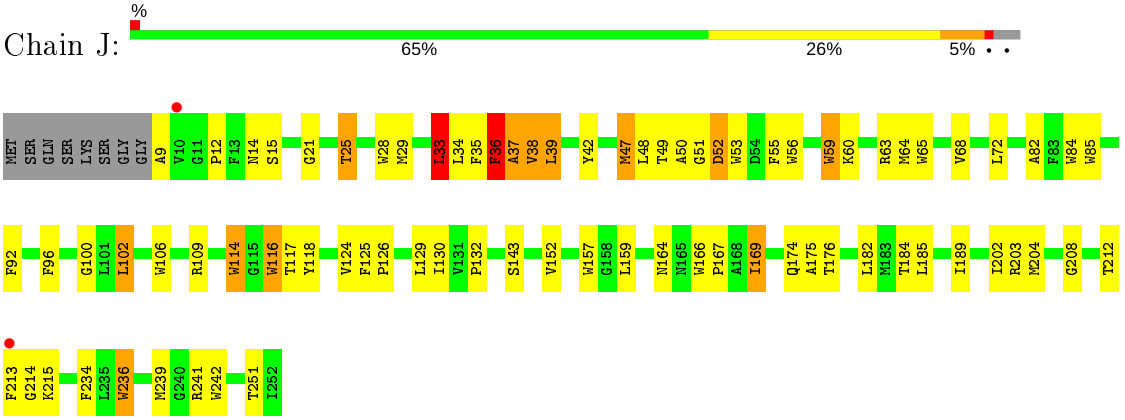
• Molecule 4: Particulate methane monooxygenase subunit A

Chain F:



• Molecule 4: Particulate methane monooxygenase subunit A

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.46Å 184.53Å 189.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 49.55 – 2.59	Depositor EDS
% Data completeness (in resolution range)	72.3 (50.00-2.59) 72.4 (49.55-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.289 0.235 , 0.286	Depositor DCC
R_{free} test set	4678 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	20853	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: PGT, 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
2	C	0.73	8/1796 (0.4%)	0.70	0/2449
2	G	0.73	5/1785 (0.3%)	0.73	1/2434 (0.0%)
2	K	0.77	5/1792 (0.3%)	0.74	1/2444 (0.0%)
3	A	0.68	5/3103 (0.2%)	0.79	2/4227 (0.0%)
3	E	0.77	4/3103 (0.1%)	0.84	0/4227
3	I	0.70	4/3103 (0.1%)	0.82	0/4227
4	B	0.82	8/2052 (0.4%)	0.81	1/2814 (0.0%)
4	F	0.93	9/2052 (0.4%)	0.84	1/2814 (0.0%)
4	J	0.95	10/2052 (0.5%)	0.88	4/2814 (0.1%)
All	All	0.78	58/20838 (0.3%)	0.80	10/28450 (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
3	A	0	1
3	E	0	2
3	I	0	2
4	B	0	1
4	F	0	2
4	J	0	2
All	All	0	10

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	242	TRP	CD2-CE2	6.74	1.49	1.41
4	J	85	TRP	CD2-CE2	6.55	1.49	1.41
4	F	236	TRP	CD2-CE2	6.54	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	132	TRP	CD2-CE2	6.49	1.49	1.41
3	I	187	TRP	CD2-CE2	6.46	1.49	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	84	LEU	CA-CB-CG	-6.87	99.50	115.30
4	B	33	LEU	CA-CB-CG	6.59	130.47	115.30
4	F	33	LEU	CA-CB-CG	6.54	130.35	115.30
3	A	260	LEU	CA-CB-CG	6.48	130.20	115.30
4	J	33	LEU	CA-CB-CG	6.29	129.76	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	333	THR	Peptide
4	B	36	PHE	Peptide
3	E	274	GLU	Peptide
3	E	333	THR	Peptide
3	I	274	GLU	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	D	95	0	22	0	0
1	H	100	0	23	2	0
1	N	120	0	28	5	0
2	C	1742	0	1749	68	0
2	G	1731	0	1737	66	0
2	K	1738	0	1746	158	0
3	A	3026	0	3015	103	0
3	E	3026	0	3015	110	0
3	I	3026	0	3015	88	0
4	B	1974	0	1932	67	0
4	F	1974	0	1932	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	1974	0	1932	70	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
6	C	51	0	78	4	0
6	G	102	0	156	7	0
6	K	51	0	78	94	0
7	A	13	0	0	4	0
7	B	11	0	0	1	0
7	C	4	0	0	2	0
7	E	25	0	0	9	0
7	F	18	0	0	1	0
7	G	11	0	0	1	0
7	I	12	0	0	0	0
7	J	16	0	0	2	0
7	K	7	0	0	4	0
All	All	20853	0	20458	734	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 18.

The worst 5 of 734 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)
2:K:84:LEU:HD13	6:K:302:PGT:C36	1.15	1.53
2:K:84:LEU:CD2	6:K:302:PGT:H341	1.42	1.47
2:K:84:LEU:CD1	6:K:302:PGT:H362	0.99	1.46
2:K:81:ALA:HA	6:K:302:PGT:C40	1.57	1.32
2:K:84:LEU:HD13	6:K:302:PGT:C35	1.58	1.31

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	210/256 (82%)	180 (86%)	25 (12%)	5 (2%)	6 10
2	G	208/256 (81%)	184 (88%)	21 (10%)	3 (1%)	11 22
2	K	209/256 (82%)	181 (87%)	26 (12%)	2 (1%)	15 32
3	A	386/420 (92%)	339 (88%)	34 (9%)	13 (3%)	3 5
3	E	386/420 (92%)	339 (88%)	32 (8%)	15 (4%)	3 4
3	I	386/420 (92%)	334 (86%)	39 (10%)	13 (3%)	3 5
4	B	242/252 (96%)	212 (88%)	27 (11%)	3 (1%)	13 27
4	F	242/252 (96%)	213 (88%)	25 (10%)	4 (2%)	9 18
4	J	242/252 (96%)	216 (89%)	24 (10%)	2 (1%)	19 39
All	All	2511/2784 (90%)	2198 (88%)	253 (10%)	60 (2%)	6 10

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	251	VAL
3	A	164	ASP
3	A	274	GLU
3	A	335	LYS
3	A	350	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	182/213 (85%)	172 (94%)	10 (6%)	21	43
2	G	181/213 (85%)	171 (94%)	10 (6%)	21	43
2	K	182/213 (85%)	170 (93%)	12 (7%)	16	33
3	A	319/336 (95%)	303 (95%)	16 (5%)	24	47
3	E	319/336 (95%)	298 (93%)	21 (7%)	16	33
3	I	319/336 (95%)	298 (93%)	21 (7%)	16	33
4	B	202/208 (97%)	185 (92%)	17 (8%)	11	21
4	F	202/208 (97%)	185 (92%)	17 (8%)	11	21
4	J	202/208 (97%)	185 (92%)	17 (8%)	11	21
All	All	2108/2271 (93%)	1967 (93%)	141 (7%)	16	33

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	368	GLN
3	I	253	THR
2	C	226	TRP
3	E	388	ILE
3	I	97	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	137	GLN
3	E	368	GLN
4	J	178	GLN
3	E	289	ASN
3	I	29	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	PGT	G	302	-	50,50,50	1.31	4 (8%)	53,56,56	1.15	2 (3%)
6	PGT	C	302	-	50,50,50	1.21	4 (8%)	53,56,56	1.04	2 (3%)
6	PGT	G	303	-	50,50,50	1.29	4 (8%)	53,56,56	1.07	4 (7%)
6	PGT	K	302	-	50,50,50	1.42	5 (10%)	53,56,56	0.97	1 (1%)

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
6	PGT	G	302	-	-	22/55/55/55	-
6	PGT	C	302	-	-	32/55/55/55	-
6	PGT	G	303	-	-	31/55/55/55	-
6	PGT	K	302	-	-	28/55/55/55	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	302	PGT	O3-C11	4.27	1.45	1.33
6	G	303	PGT	O2-C31	3.87	1.45	1.34
6	G	303	PGT	O3-C11	3.82	1.44	1.33
6	C	302	PGT	O3-C11	3.80	1.44	1.33
6	G	302	PGT	O2-C31	3.68	1.44	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	302	PGT	O2-C31-C32	4.68	121.58	111.50
6	G	303	PGT	O2-C31-C32	3.88	119.87	111.50
6	G	302	PGT	O2-C31-O31	-3.57	115.08	123.70
6	K	302	PGT	O2-C31-C32	3.30	118.61	111.50
6	C	302	PGT	O2-C31-C32	3.25	118.51	111.50

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	PGT	C32-C31-O2-C2
6	C	302	PGT	O2-C2-C3-O3
6	C	302	PGT	C1-O3P-P-O1P
6	C	302	PGT	C1-O3P-P-O2P
6	C	302	PGT	C1-O3P-P-O4P

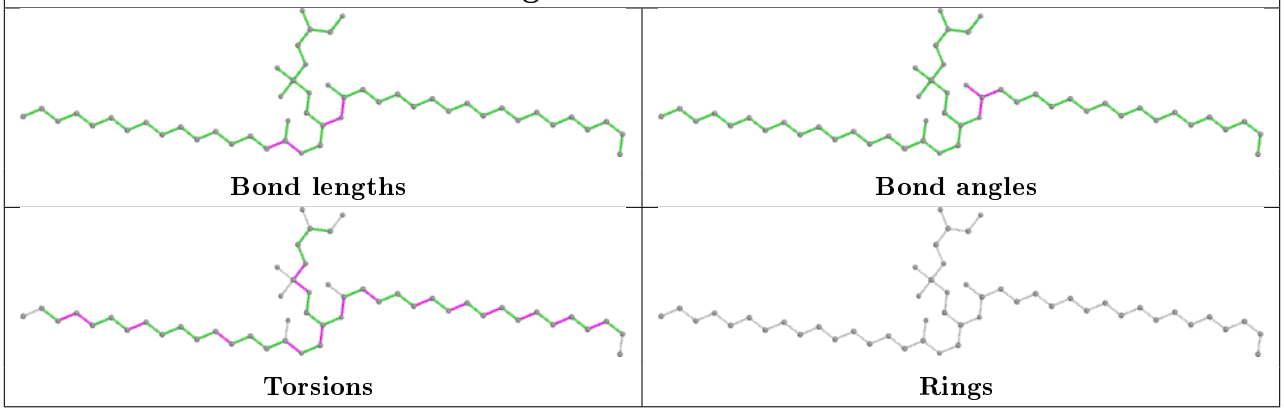
There are no ring outliers.

4 monomers are involved in 105 short contacts:

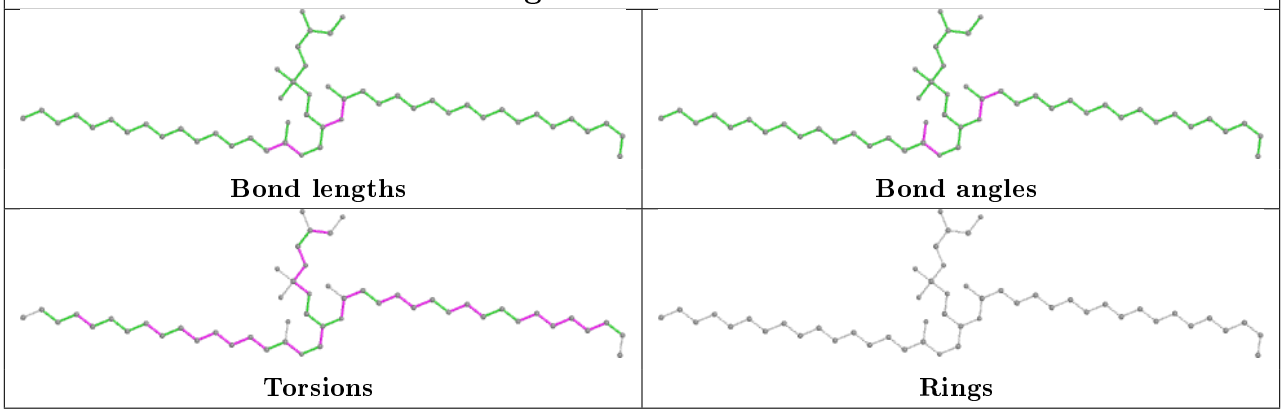
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	302	PGT	2	0
6	C	302	PGT	4	0
6	G	303	PGT	5	0
6	K	302	PGT	94	0

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.

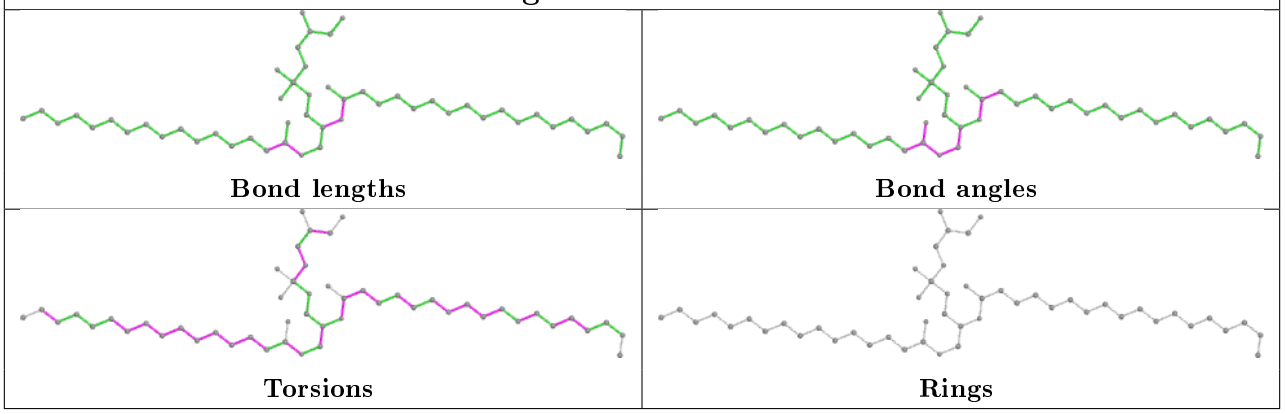
Ligand PGT G 302

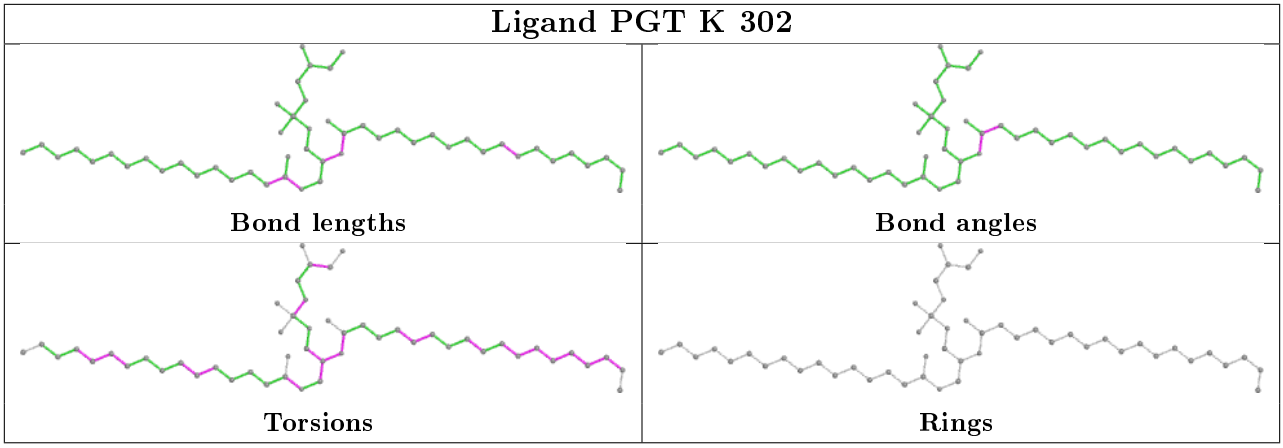


Ligand PGT C 302



Ligand PGT G 303





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	D	0/24	-	-	-	-
1	H	0/24	-	-	-	-
1	N	0/24	-	-	-	-
2	C	214/256 (83%)	0.39	15 (7%) 16 12	26, 51, 93, 124	0
2	G	212/256 (82%)	0.28	17 (8%) 12 9	22, 46, 86, 112	0
2	K	213/256 (83%)	0.18	14 (6%) 18 13	14, 37, 92, 120	0
3	A	388/420 (92%)	0.28	25 (6%) 19 14	18, 49, 82, 105	0
3	E	388/420 (92%)	-0.21	8 (2%) 63 58	7, 28, 55, 82	0
3	I	388/420 (92%)	0.32	34 (8%) 10 7	18, 43, 83, 141	0
4	B	244/252 (96%)	-0.03	9 (3%) 41 34	24, 39, 71, 123	0
4	F	244/252 (96%)	-0.16	3 (1%) 79 76	10, 24, 63, 93	0
4	J	244/252 (96%)	-0.31	2 (0%) 86 84	11, 24, 52, 88	0
All	All	2535/2856 (88%)	0.08	127 (5%) 28 23	7, 37, 80, 141	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	252	LYS	10.0
3	I	350	VAL	9.9
2	K	252	LYS	9.2
2	G	253	LEU	7.9
2	C	17	SER	7.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

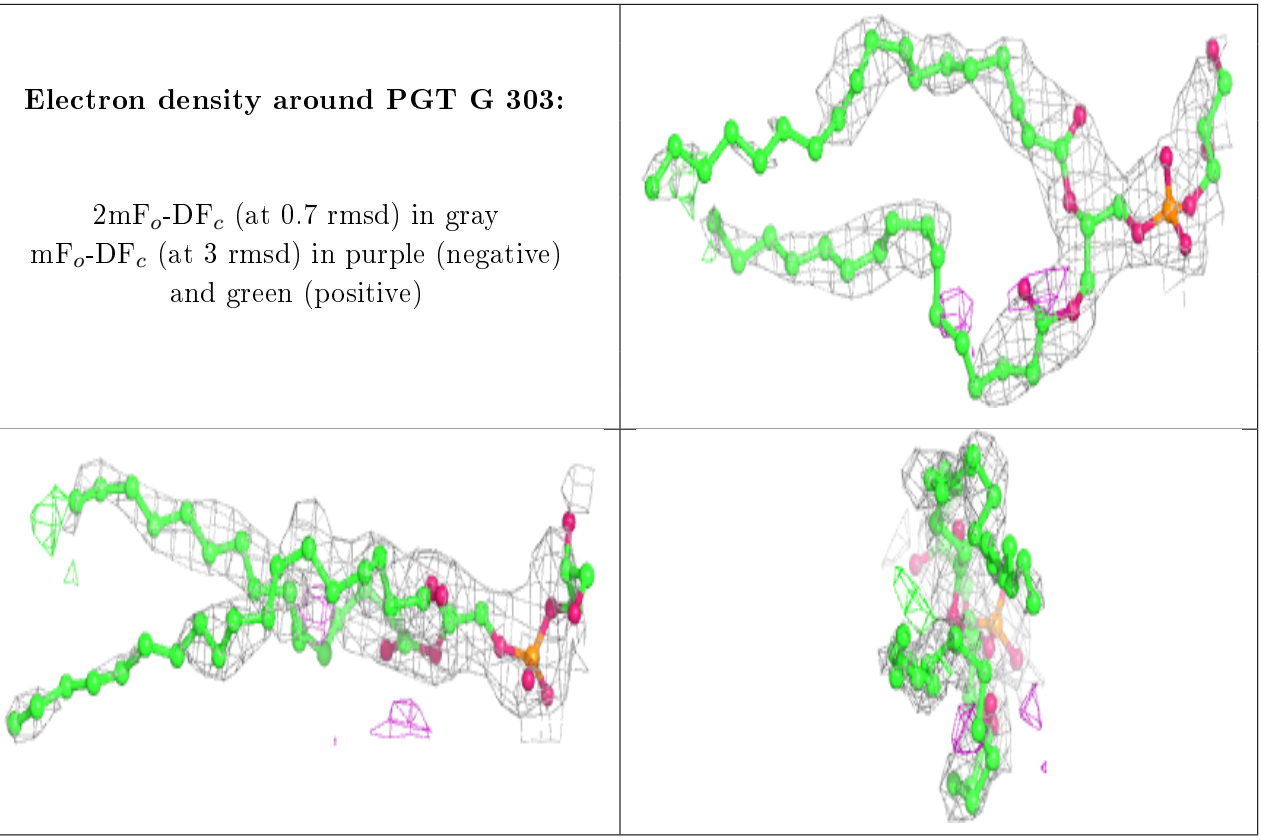
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	PGT	G	303	51/51	0.81	0.33	53,71,114,115	0
6	PGT	C	302	51/51	0.86	0.34	51,75,90,95	0
6	PGT	G	302	51/51	0.89	0.34	45,59,99,106	0
6	PGT	K	302	51/51	0.89	0.26	24,39,51,53	0
5	CU	A	501	1/1	0.97	0.10	49,49,49,49	1
5	CU	C	301	1/1	0.98	0.04	62,62,62,62	1
5	CU	G	301	1/1	0.98	0.07	70,70,70,70	1
5	CU	I	501	1/1	0.99	0.07	60,60,60,60	0
5	CU	K	301	1/1	0.99	0.05	62,62,62,62	1
5	CU	E	501	1/1	1.00	0.10	24,24,24,24	1

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.

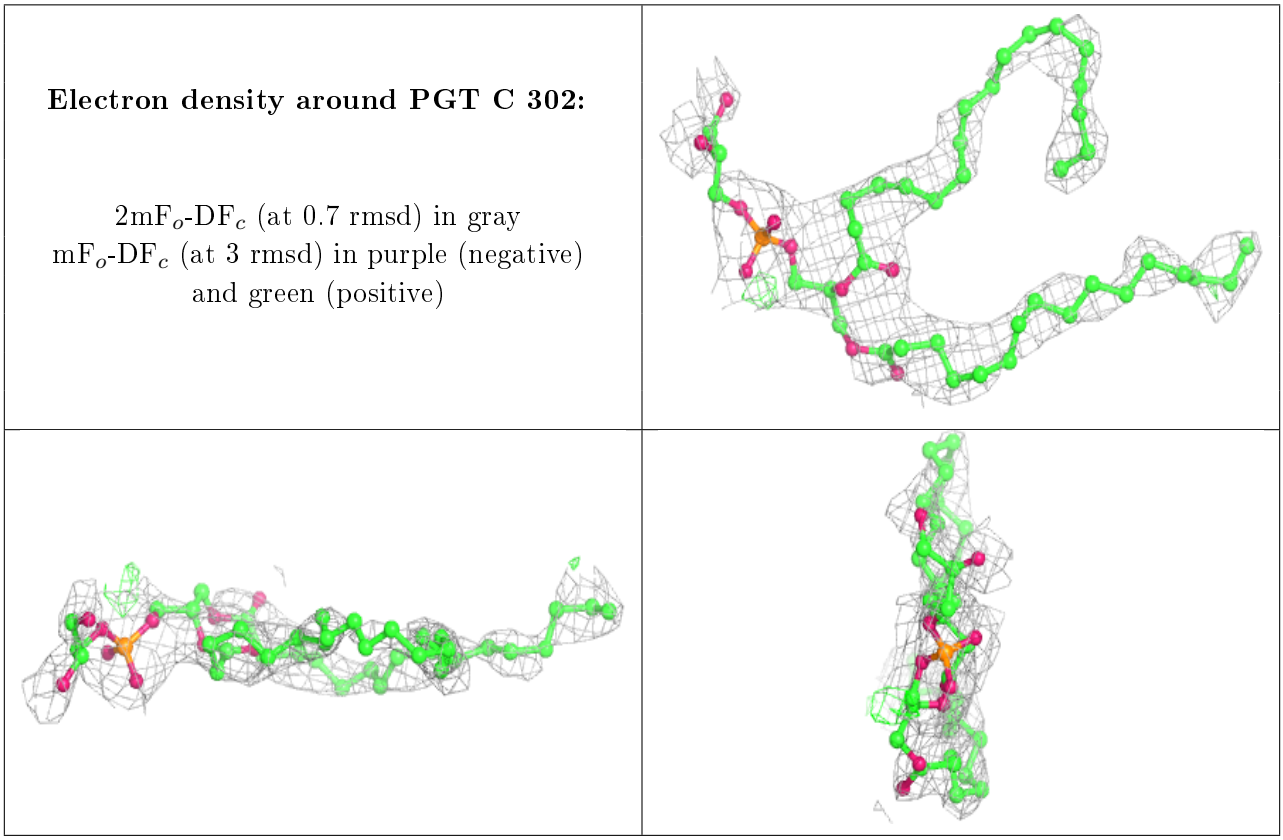
Electron density around PGT G 303:

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



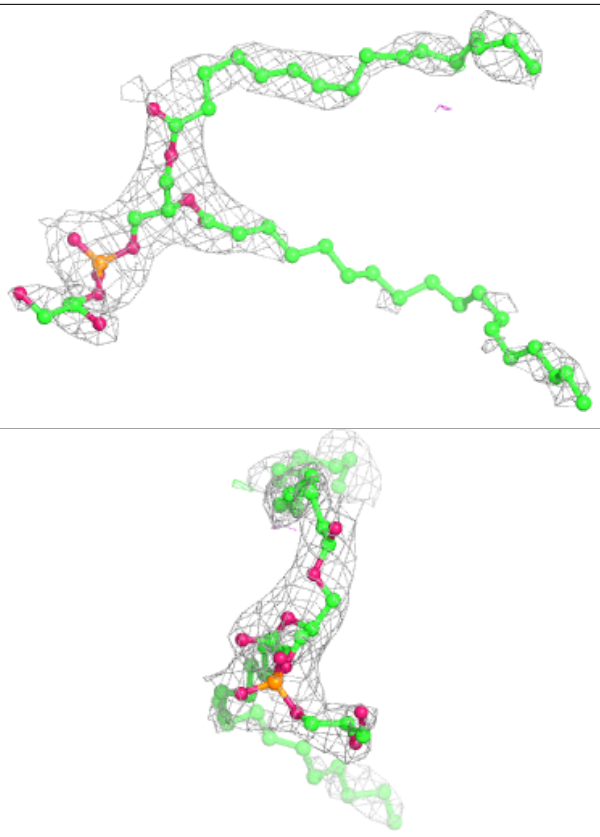
Electron density around PGT C 302:

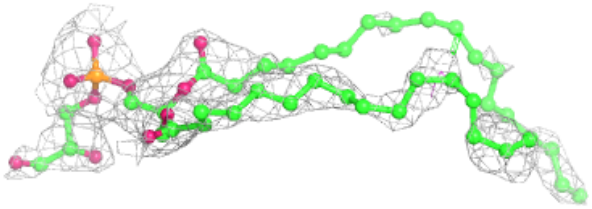
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PGT G 302:

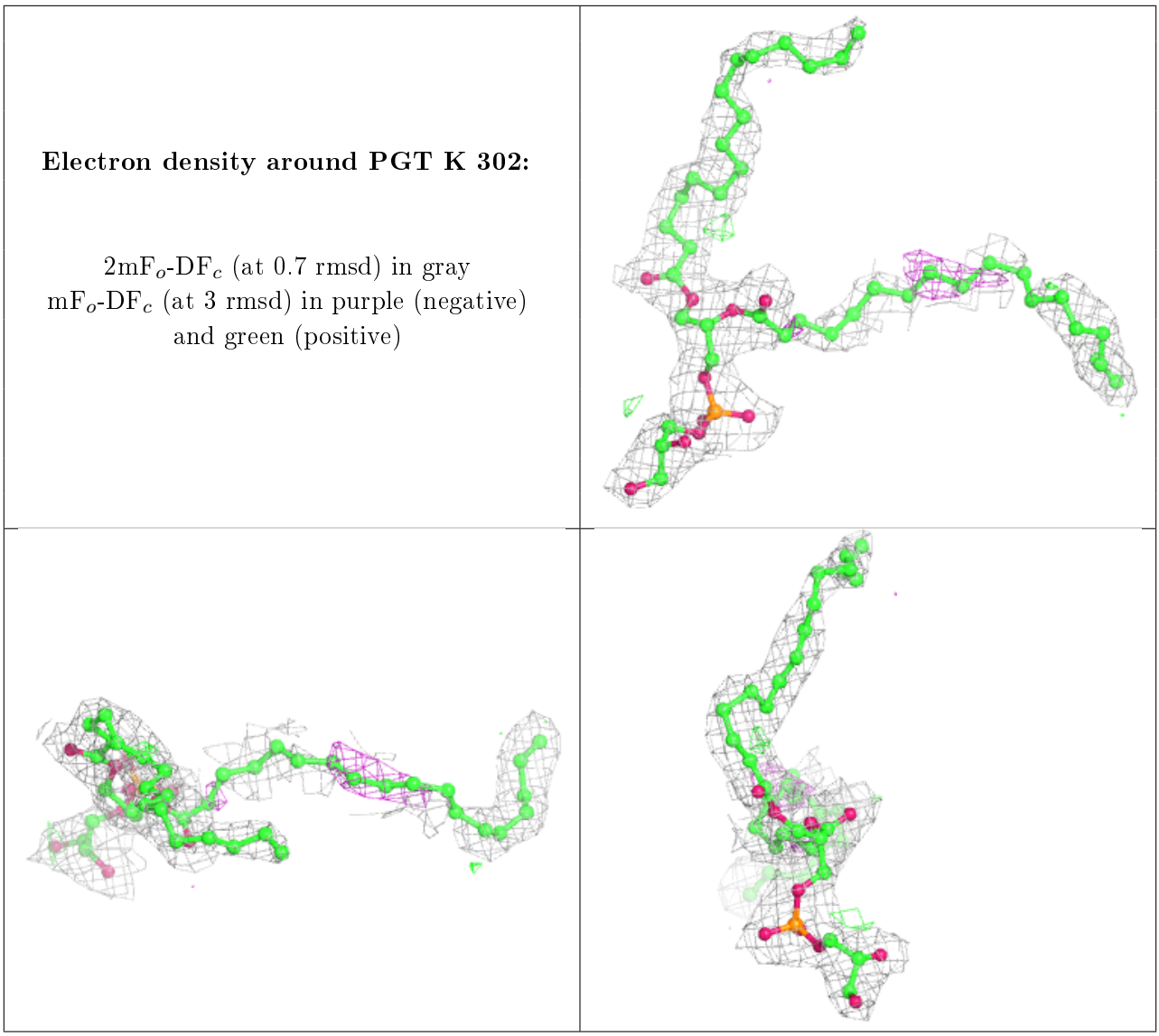
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around PGT K 302:

$2mF_o$-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.