wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 10:12 PM EDT

PDB ID	:	3SQG / pdb_00003sqg
Title	:	Crystal structure of a methyl-coenzyme M reductase purified from Black Sea mats
Authors	:	Shima, S.; Krueger, M.; Weinert, T.; Demmer, U.; Thauer, R.K.; Ermler, U.
Deposited on	:	2011-07-05
Resolution	:	2.10 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:

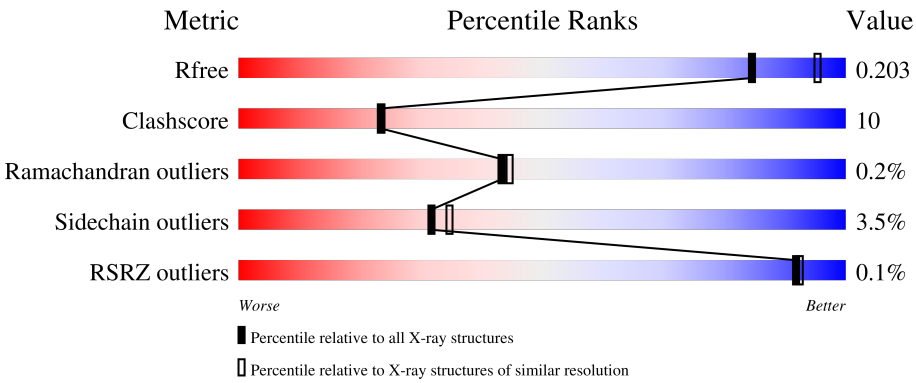
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	579	82% 16% •
1	D	579	83% 16% •
1	G	579	85% 13% •
2	B	433	80% 18% •
2	E	433	76% 22% •

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Mol	Chain	Length	Quality of chain
2	H	433	79% 18% •
3	C	279	87% 12% •
3	F	279	79% 19% •
3	I	279	84% 14% •

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
1	GL3	A	464	-	-	X	-
10	CL	A	586	-	-	X	-
12	P6G	B	434	-	-	X	-
5	COM	A	1003	-	X	X	-
6	M43	D	1001	X	-	-	-
6	M43	G	1001	X	-	-	-
7	1PE	D	580	-	-	X	-
7	1PE	G	580	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 32144 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 Methyl coenzyme M reductase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	4467	2814	761	855	37	0	0	0
1	D	578	4475	2819	764	855	37	0	1	0
1	G	578	4467	2814	761	855	37	0	0	0

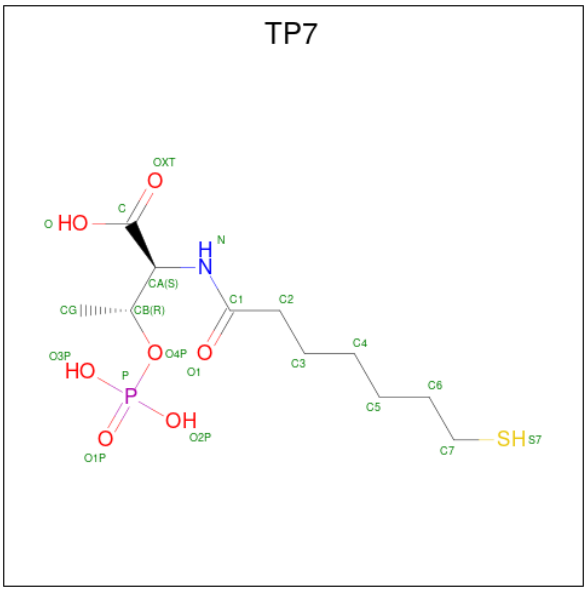
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3197	2013	552	600	32	0	0	0
2	E	431	3197	2013	552	600	32	0	0	0
2	H	431	3205	2018	555	600	32	0	1	0

- Molecule 3 is a protein called Methyl-coenzyme M reductase, gamma subunit.

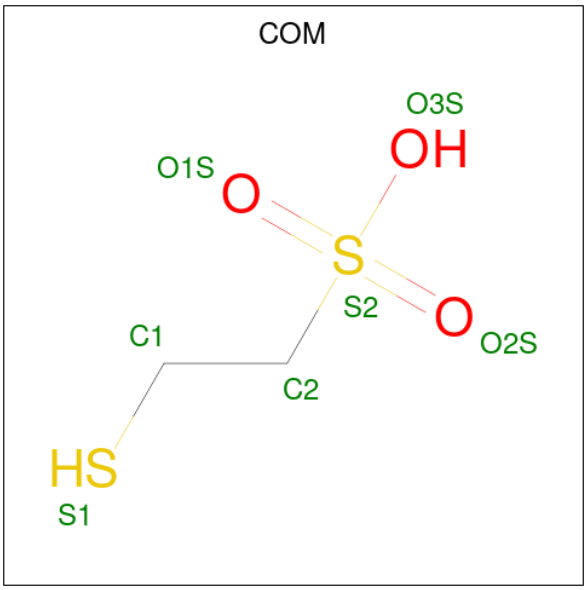
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	278	2205	1379	400	414	12	0	0	0
3	F	278	2210	1382	401	415	12	0	1	0
3	I	278	2205	1379	400	414	12	0	0	0

- Molecule 4 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	21	11	1	7	1	1	0	0
			Total	C	N	O	P	S		
4	A	1	21	11	1	7	1	1	0	0
			Total	C	N	O	P	S		
4	G	1	21	11	1	7	1	1	0	0

- Molecule 5 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	7	2	3	2	0	0

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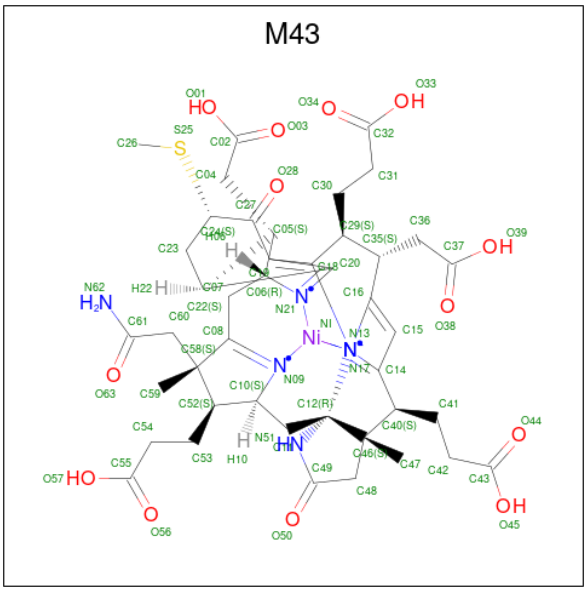
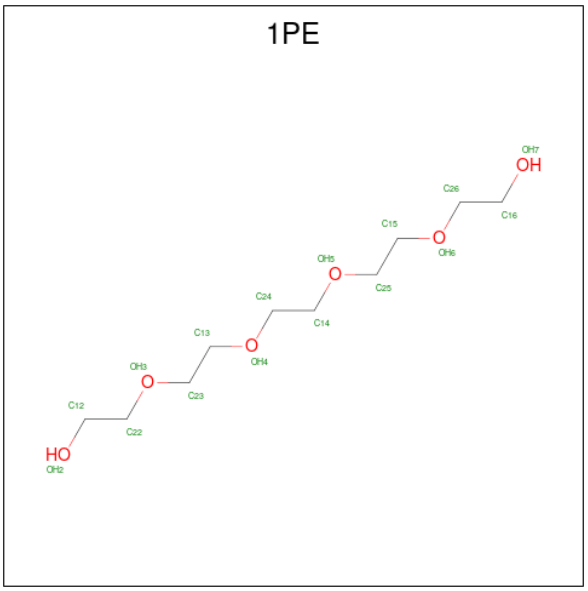
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	D	1	7	2	3	2	0	0
			Total	C	O	S		
5	G	1	7	2	3	2	0	0

- Molecule 6 is (17[2]S)-17[2]-methylthio-coenzyme F43 (CCD ID: M43) (formula: $C_{43}H_{53}N_6NiO_{13}S$).



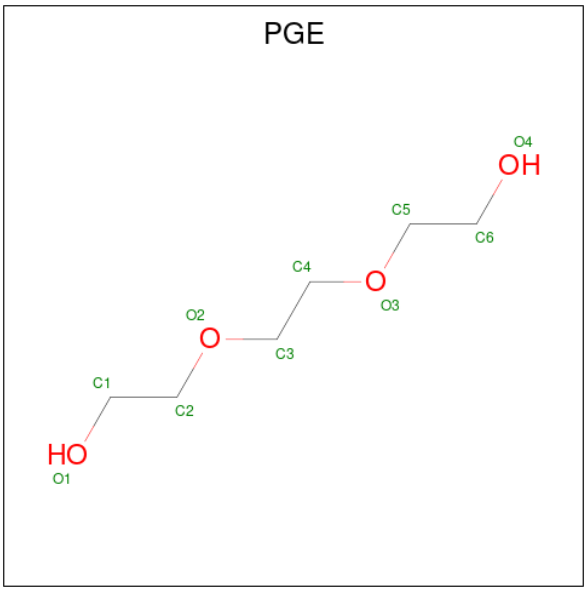
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	Ni	O	S		
6	A	1	64	43	6	1	13	1	0	0
			Total	C	N	Ni	O	S		
6	D	1	64	43	6	1	13	1	0	0
			Total	C	N	Ni	O	S		
6	G	1	64	43	6	1	13	1	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



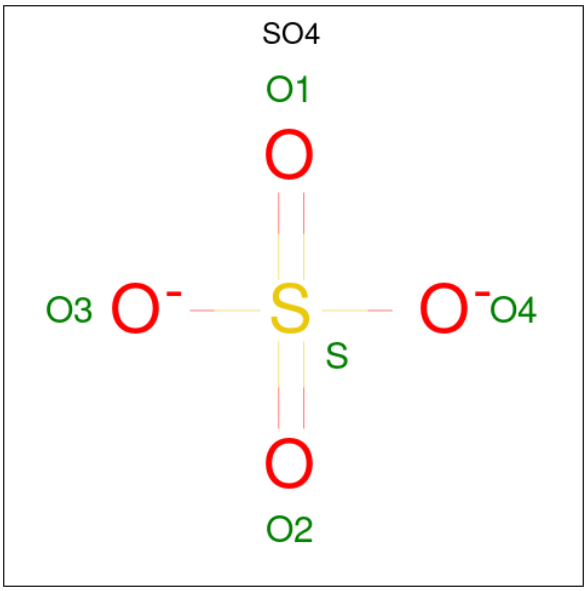
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	16	10	6	0	0
			Total	C	O		
7	D	1	16	10	6	0	0
			Total	C	O		
7	E	1	16	10	6	0	0
			Total	C	O		
7	F	1	16	10	6	0	0
			Total	C	O		
7	G	1	16	10	6	0	0
			Total	C	O		
7	H	1	16	10	6	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O		0	0
			10	6	4			
8	A	1	Total	C	O		0	0
			10	6	4			
8	D	1	Total	C	O		0	0
			10	6	4			
8	D	1	Total	C	O		0	0
			10	6	4			
8	G	1	Total	C	O		0	0
			10	6	4			
8	G	1	Total	C	O		0	0
			10	6	4			

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
9	A	1	5	4	1	0	0
			Total	O	S		
9	A	1	5	4	1	0	0
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	B	1	5	4	1	0	0
			Total	O	S		
9	C	1	5	4	1	0	0
			Total	O	S		
9	D	1	5	4	1	0	0
			Total	O	S		
9	D	1	5	4	1	0	0
			Total	O	S		
9	H	1	5	4	1	0	0
			Total	O	S		
9	I	1	5	4	1	0	0

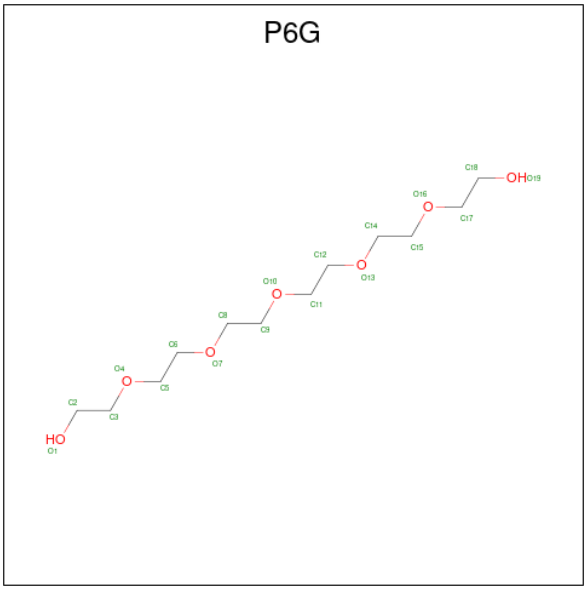
- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
10	A	1	1	1	0	0

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

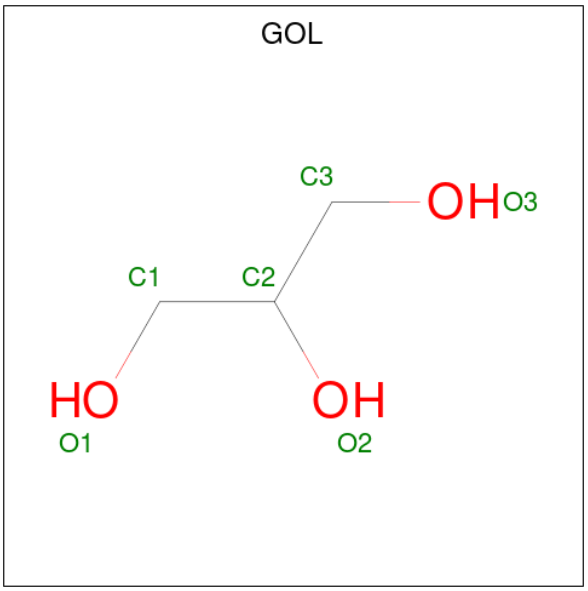
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Ca 1 1	0	0
11	G	1	Total Ca 1 1	0	0

- Molecule 12 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 19 12 7	0	0

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	C	1	6	3	3	0	0
			Total	C	O		
13	E	1	6	3	3	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	391	391	391	0	0
			Total	O		
14	B	173	173	173	0	0
			Total	O		
14	C	178	178	178	0	0
			Total	O		
14	D	341	341	341	0	0
			Total	O		
14	E	142	142	142	0	0
			Total	O		
14	F	120	120	120	0	0
			Total	O		
14	G	364	364	364	0	0
			Total	O		
14	H	140	140	140	0	0
			Total	O		
14	I	156	156	156	0	0

3 Residue-property plots (i)

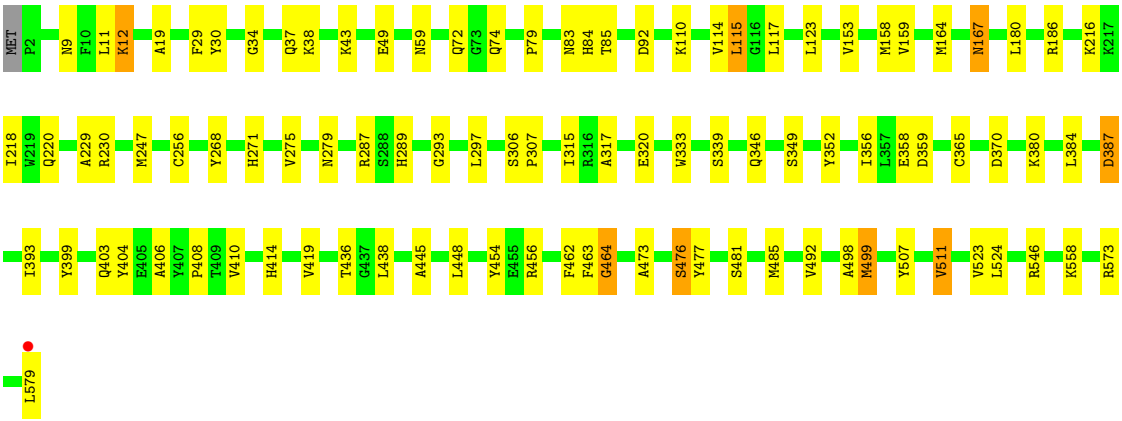
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Methyl coenzyme M reductase, alpha subunit

Chain A:

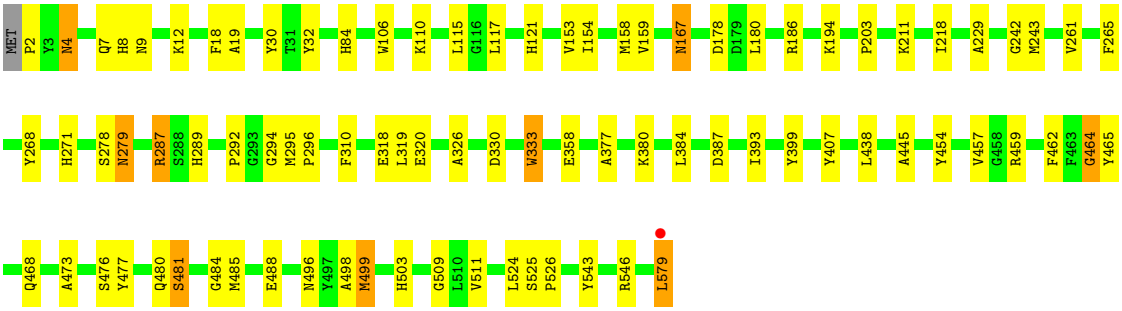
• Molecule 1: Methyl coenzyme M reductase, alpha subunit

Chain D:



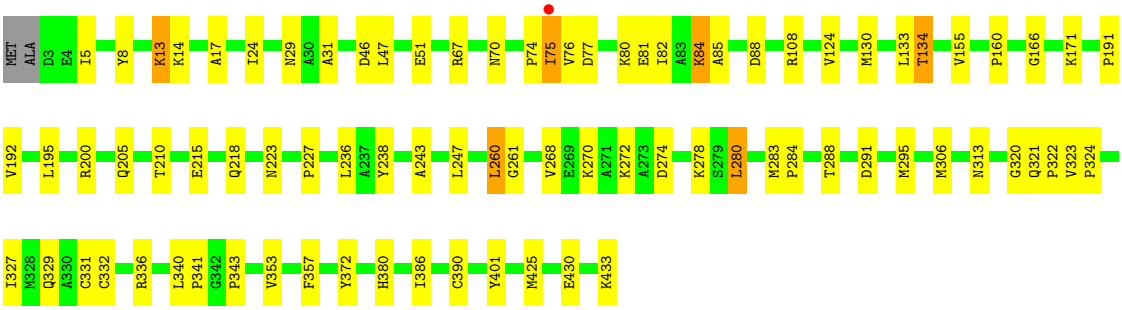
• Molecule 1: Methyl coenzyme M reductase, alpha subunit

Chain G:



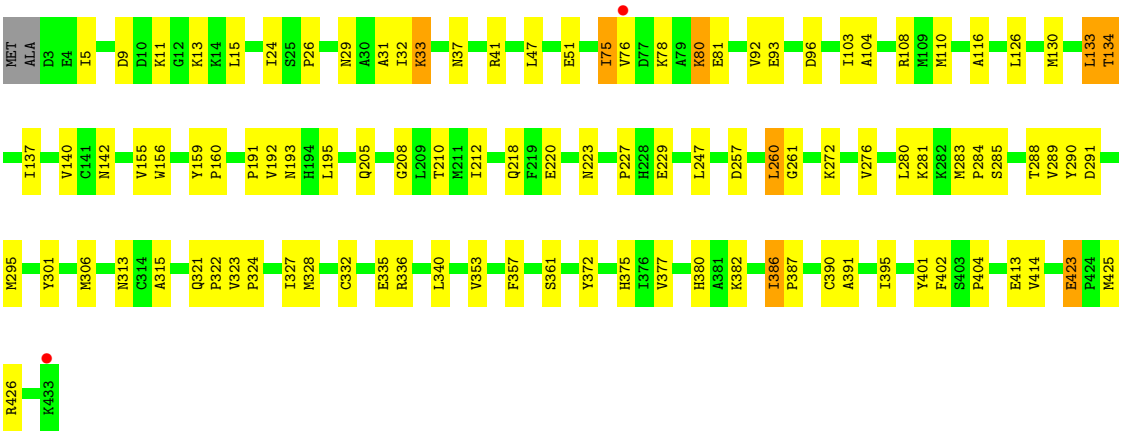
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain B:



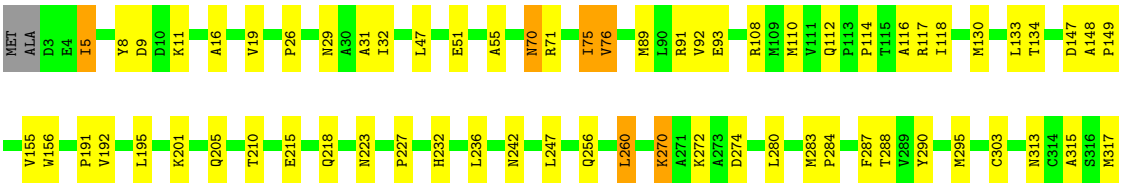
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain E:



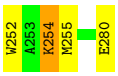
- Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain H:



• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain C:

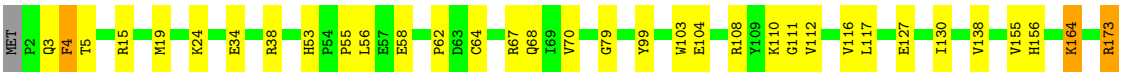


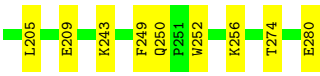
• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain F:

• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain I:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	128.86Å 412.49Å 165.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.10 47.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.58-2.10) 95.3 (47.58-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.161 , 0.206 0.157 , 0.203	Depositor DCC
R_{free} test set	12184 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32144	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: 1PE, CA, P6G, TP7, SO4, PGE, GL3, GOL, 0AF, MHO, CL, M43, MHS, COM

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	0.54	0/4528	0.79	1/6126 (0.0%)
1	D	0.50	0/4539	0.77	0/6140
1	G	0.49	0/4528	0.78	2/6126 (0.0%)
2	B	0.46	0/3258	0.77	1/4410 (0.0%)
2	E	0.42	0/3258	0.78	3/4410 (0.1%)
2	H	0.45	1/3269 (0.0%)	0.80	2/4424 (0.0%)
3	C	0.48	0/2251	0.78	0/3034
3	F	0.38	0/2259	0.74	2/3045 (0.1%)
3	I	0.45	0/2251	0.76	0/3034
All	All	0.47	1/30141 (0.0%)	0.78	11/40749 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	323	VAL	CA-CB	5.88	1.57	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	118	ILE	N-CA-C	6.24	112.89	106.21
3	F	250	GLN	CA-C-N	6.14	126.33	119.32
3	F	250	GLN	C-N-CA	6.14	126.33	119.32
2	B	380	HIS	N-CA-C	5.48	117.34	111.36
1	G	310	PHE	CA-C-N	5.37	125.19	119.28

There are no chirality outliers.

There are no planarity outliers.

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	4467	0	4267	91	0
1	D	4475	0	4280	102	0
1	G	4467	0	4267	80	0
2	B	3197	0	3195	85	0
2	E	3197	0	3195	105	0
2	H	3205	0	3208	98	0
3	C	2205	0	2187	40	0
3	F	2210	0	2193	56	0
3	I	2205	0	2187	44	0
4	A	42	0	38	1	0
4	G	21	0	19	1	0
5	A	7	0	5	4	0
5	D	7	0	5	3	0
5	G	7	0	5	3	0
6	A	64	0	48	3	0
6	D	64	0	48	1	0
6	G	64	0	48	3	0
7	A	16	0	22	5	0
7	D	16	0	22	8	0
7	E	16	0	22	2	0
7	F	16	0	22	4	0
7	G	16	0	22	9	0
7	H	16	0	22	5	0
8	A	20	0	28	5	0
8	D	20	0	28	5	0
8	G	20	0	28	1	0
9	A	10	0	0	0	0
9	B	10	0	0	0	0
9	C	5	0	0	0	0
9	D	10	0	0	0	0
9	H	5	0	0	0	0
9	I	5	0	0	0	0
10	A	1	0	0	3	0
11	A	1	0	0	0	0
11	G	1	0	0	0	0
12	B	19	0	26	11	0
13	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	E	6	0	8	0	0
14	A	391	0	0	6	0
14	B	173	0	0	7	0
14	C	178	0	0	4	0
14	D	341	0	0	9	0
14	E	142	0	0	7	0
14	F	120	0	0	4	0
14	G	364	0	0	2	0
14	H	140	0	0	2	0
14	I	156	0	0	1	0
All	All	32144	0	29453	609	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 10.

The worst 5 of 609 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:B:51:GLU:HB2	2:B:75:ILE:CD1	1.77	1.15
1:D:186:ARG:HH12	7:G:580:1PE:H221	1.16	1.10
2:B:14:LYS:CE	2:B:17:ALA:HB2	1.86	1.06
1:A:186:ARG:HH12	7:A:581:1PE:H121	1.20	1.03
7:D:580:1PE:H141	1:G:186:ARG:HH11	1.25	1.02

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	572/579 (99%)	547 (96%)	23 (4%)	2 (0%)	36 36
1	D	573/579 (99%)	545 (95%)	26 (4%)	2 (0%)	36 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	572/579 (99%)	547 (96%)	24 (4%)	1 (0%)	43	44
2	B	429/433 (99%)	421 (98%)	8 (2%)	0	100	100
2	E	429/433 (99%)	418 (97%)	11 (3%)	0	100	100
2	H	430/433 (99%)	417 (97%)	13 (3%)	0	100	100
3	C	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	28
3	F	277/279 (99%)	269 (97%)	8 (3%)	0	100	100
3	I	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	30	28
All	All	3834/3873 (99%)	3698 (96%)	129 (3%)	7 (0%)	43	44

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	481	SER
1	A	481	SER
1	D	481	SER
3	I	4	PHE
1	A	339	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	453/454 (100%)	434 (96%)	19 (4%)	26	28
1	D	454/454 (100%)	437 (96%)	17 (4%)	30	33
1	G	453/454 (100%)	438 (97%)	15 (3%)	33	37
2	B	331/332 (100%)	317 (96%)	14 (4%)	26	28
2	E	331/332 (100%)	320 (97%)	11 (3%)	33	37
2	H	332/332 (100%)	322 (97%)	10 (3%)	36	41
3	C	231/232 (100%)	224 (97%)	7 (3%)	36	41
3	F	232/232 (100%)	224 (97%)	8 (3%)	32	35
3	I	231/232 (100%)	226 (98%)	5 (2%)	45	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3048/3054 (100%)	2942 (96%)	106 (4%)	32 35

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	5	ILE
3	F	60	GLU
2	H	270	LYS
2	E	75	ILE
2	E	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	3	GLN
1	G	279	ASN
3	F	226	GLN
1	G	84	HIS
1	G	468	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	GL3	A	464	1	2,3,4	2.98	1 (50%)	1,2,4	0.47	0
1	MHO	G	499	1	6,8,9	0.76	0	3,9,11	2.38	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	0AF	D	333	1	15,16,17	1.03	1 (6%)	14,22,24	1.20	2 (14%)
1	GL3	D	464	1	2,3,4	2.80	1 (50%)	1,2,4	0.12	0
1	MHS	G	271	1	10,11,12	1.39	2 (20%)	5,14,16	3.08	1 (20%)
1	MHO	D	499	1	6,8,9	0.74	0	3,9,11	1.69	1 (33%)
1	0AF	G	333	1	15,16,17	1.06	1 (6%)	14,22,24	1.11	2 (14%)
1	GL3	G	464	1	2,3,4	2.60	1 (50%)	1,2,4	0.25	0
1	0AF	A	333	1	15,16,17	1.02	2 (13%)	14,22,24	1.27	2 (14%)
1	MHO	A	499	1	6,8,9	0.63	0	3,9,11	1.64	1 (33%)
1	MHS	A	271	1	10,11,12	1.07	0	5,14,16	3.89	2 (40%)
1	MHS	D	271	1	10,11,12	1.28	1 (10%)	5,14,16	3.02	1 (20%)

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
1	GL3	A	464	1	-	0/1/1/2	-
1	MHO	G	499	1	-	3/6/7/9	-
1	0AF	D	333	1	-	0/5/6/8	0/2/2/2
1	GL3	D	464	1	-	1/1/1/2	-
1	MHS	G	271	1	-	0/5/6/8	0/1/1/1
1	MHO	D	499	1	-	3/6/7/9	-
1	0AF	G	333	1	-	0/5/6/8	0/2/2/2
1	GL3	G	464	1	-	1/1/1/2	-
1	0AF	A	333	1	-	0/5/6/8	0/2/2/2
1	MHO	A	499	1	-	3/6/7/9	-
1	MHS	A	271	1	-	0/5/6/8	0/1/1/1
1	MHS	D	271	1	-	0/5/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	GL3	C-S	-4.17	1.63	1.80
1	D	464	GL3	C-S	-3.89	1.64	1.80
1	G	464	GL3	C-S	-3.57	1.66	1.80
1	D	333	0AF	CD1-NE1	2.65	1.41	1.37
1	G	271	MHS	CD2-CG	2.49	1.40	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	MHS	ND1-CE1-NE2	-7.96	108.20	112.94
1	G	271	MHS	ND1-CE1-NE2	-6.47	109.09	112.94
1	D	271	MHS	ND1-CE1-NE2	-6.29	109.19	112.94
1	A	333	0AF	CE2-NE1-CD1	-2.97	106.37	108.93
1	G	499	MHO	CE-SD-CG	-2.97	90.04	97.45

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-CE
1	D	499	MHO	O-C-CA-CB
1	G	499	MHO	O-C-CA-CB
1	A	499	MHO	CB-CG-SD-OD1

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	464	GL3	4	0
1	G	499	MHO	2	0
1	D	464	GL3	3	0
1	D	499	MHO	1	0
1	G	333	0AF	1	0
1	G	464	GL3	3	0
1	A	499	MHO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
9	SO4	B	436	-	4,4,4	0.24	0	6,6,6	0.23	0
9	SO4	D	583	-	4,4,4	0.24	0	6,6,6	0.12	0
4	TP7	G	1002	-	19,20,20	2.79	2 (10%)	24,26,26	2.32	5 (20%)
7	1PE	D	580	-	15,15,15	0.67	0	14,14,14	1.55	2 (14%)
9	SO4	D	584	-	4,4,4	0.24	0	6,6,6	0.10	0
6	M43	G	1001	5,1	64,73,73	3.37	25 (39%)	71,121,121	2.18	12 (16%)
13	GOL	E	435	-	5,5,5	0.41	0	5,5,5	0.23	0
5	COM	G	1003	6	6,6,6	3.06	1 (16%)	8,8,8	1.59	2 (25%)
13	GOL	C	281	-	5,5,5	0.44	0	5,5,5	0.50	0
9	SO4	A	585	-	4,4,4	0.25	0	6,6,6	0.07	0
8	PGE	G	582	-	9,9,9	0.51	0	8,8,8	0.18	0
5	COM	D	1003	6	6,6,6	2.86	1 (16%)	8,8,8	2.01	2 (25%)
6	M43	A	1001	5,1	64,73,73	3.51	25 (39%)	71,121,121	2.38	15 (21%)
9	SO4	H	435	-	4,4,4	0.23	0	6,6,6	0.10	0
9	SO4	B	435	-	4,4,4	0.24	0	6,6,6	0.09	0
9	SO4	C	282	-	4,4,4	0.24	0	6,6,6	0.20	0
7	1PE	A	581	-	15,15,15	0.65	0	14,14,14	1.52	0
8	PGE	D	581	-	9,9,9	0.53	0	8,8,8	0.28	0
5	COM	A	1003	6	6,6,6	2.80	1 (16%)	8,8,8	3.12	3 (37%)
12	P6G	B	434	-	18,18,18	0.71	0	17,17,17	1.52	0
7	1PE	H	434	-	15,15,15	0.68	0	14,14,14	1.58	3 (21%)
6	M43	D	1001	5,1	64,73,73	3.67	26 (40%)	71,121,121	2.21	13 (18%)
4	TP7	A	580	-	19,20,20	2.73	2 (10%)	24,26,26	2.38	5 (20%)
7	1PE	F	281	-	15,15,15	0.65	0	14,14,14	1.58	3 (21%)
8	PGE	G	581	-	9,9,9	0.51	0	8,8,8	0.21	0
7	1PE	G	580	-	15,15,15	0.58	0	14,14,14	1.65	3 (21%)
8	PGE	A	583	-	9,9,9	0.54	0	8,8,8	0.36	0
9	SO4	A	584	-	4,4,4	0.24	0	6,6,6	0.15	0
8	PGE	D	582	-	9,9,9	0.54	0	8,8,8	0.25	0
7	1PE	E	434	-	15,15,15	0.69	0	14,14,14	1.49	2 (14%)
9	SO4	I	281	-	4,4,4	0.22	0	6,6,6	0.10	0
8	PGE	A	582	-	9,9,9	0.41	0	8,8,8	0.43	0
4	TP7	A	1002	-	19,20,20	2.68	2 (10%)	24,26,26	2.38	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TP7	G	1002	-	-	3/24/24/24	-
7	1PE	D	580	-	-	5/13/13/13	-
6	M43	G	1001	5,1	1/1/31/33	7/28/190/190	-
13	GOL	E	435	-	-	3/4/4/4	-
5	COM	G	1003	6	-	3/4/4/4	-
13	GOL	C	281	-	-	0/4/4/4	-
8	PGE	G	582	-	-	1/7/7/7	-
5	COM	D	1003	6	-	3/4/4/4	-
6	M43	A	1001	5,1	-	9/28/190/190	-
7	1PE	A	581	-	-	9/13/13/13	-
8	PGE	D	581	-	-	2/7/7/7	-
5	COM	A	1003	6	-	4/4/4/4	-
12	P6G	B	434	-	-	8/16/16/16	-
7	1PE	H	434	-	-	7/13/13/13	-
6	M43	D	1001	5,1	1/1/31/33	10/28/190/190	-
4	TP7	A	580	-	-	2/24/24/24	-
7	1PE	F	281	-	-	5/13/13/13	-
8	PGE	G	581	-	-	3/7/7/7	-
7	1PE	G	580	-	-	9/13/13/13	-
8	PGE	A	583	-	-	6/7/7/7	-
8	PGE	D	582	-	-	2/7/7/7	-
7	1PE	E	434	-	-	8/13/13/13	-
8	PGE	A	582	-	-	4/7/7/7	-
4	TP7	A	1002	-	-	3/24/24/24	-

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1001	M43	NI-N13	13.23	2.21	1.89
6	A	1001	M43	NI-N13	12.78	2.20	1.89
6	D	1001	M43	NI-N21	11.42	2.16	1.89
6	G	1001	M43	NI-N21	11.32	2.16	1.89
4	G	1002	TP7	O1-C1	10.50	1.44	1.23

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1001	M43	C59-C58-C60	13.84	134.26	110.74
6	G	1001	M43	C59-C58-C60	11.20	129.77	110.74
6	D	1001	M43	C59-C58-C60	9.80	127.39	110.74
4	A	580	TP7	O1-C1-N	-8.89	107.90	122.95
4	A	1002	TP7	O1-C1-N	-8.71	108.21	122.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	1001	M43	N17
6	G	1001	M43	N17

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	TP7	O1-C1-N-CA
4	A	580	TP7	O1-C1-N-CA
4	G	1002	TP7	O1-C1-N-CA
5	A	1003	COM	C1-C2-S2-O1S
5	A	1003	COM	C1-C2-S2-O2S

There are no ring outliers.

20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1002	TP7	1	0
7	D	580	1PE	8	0
6	G	1001	M43	3	0
5	G	1003	COM	3	0
8	G	582	PGE	1	0
5	D	1003	COM	3	0
6	A	1001	M43	3	0
7	A	581	1PE	5	0
8	D	581	PGE	3	0
5	A	1003	COM	4	0
12	B	434	P6G	11	0
7	H	434	1PE	5	0
6	D	1001	M43	1	0
7	F	281	1PE	4	0
7	G	580	1PE	9	0
8	A	583	PGE	4	0
8	D	582	PGE	2	0
7	E	434	1PE	2	0

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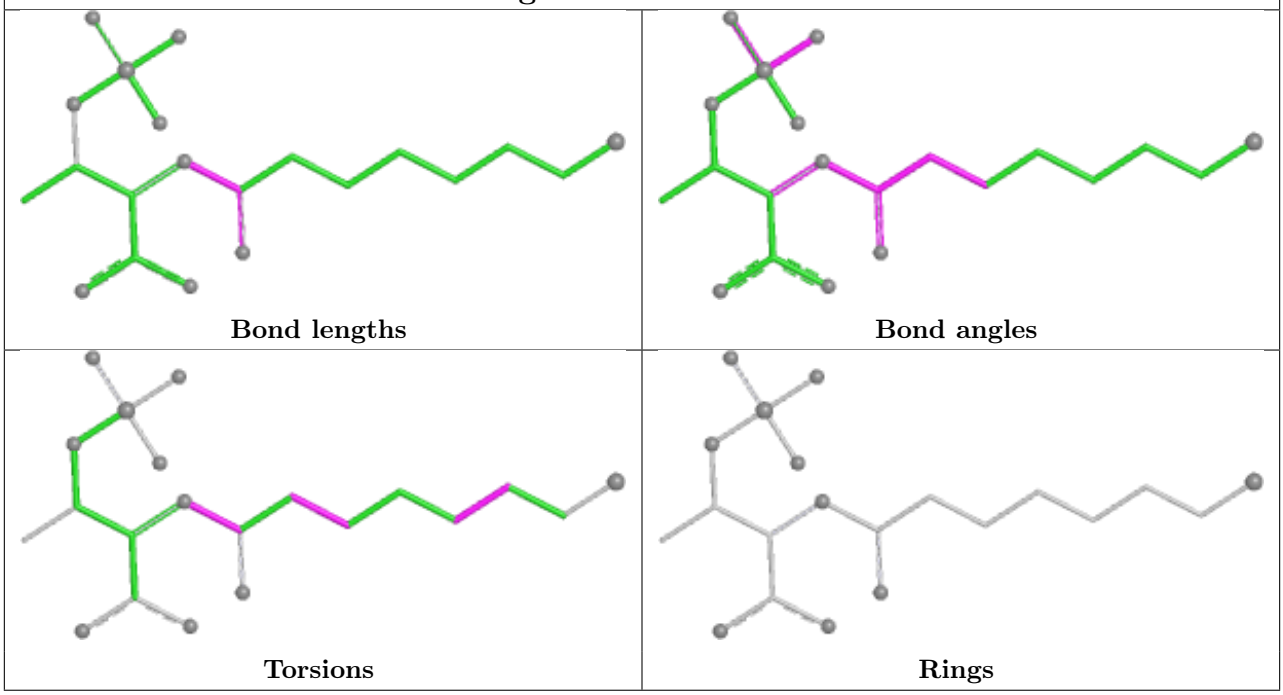
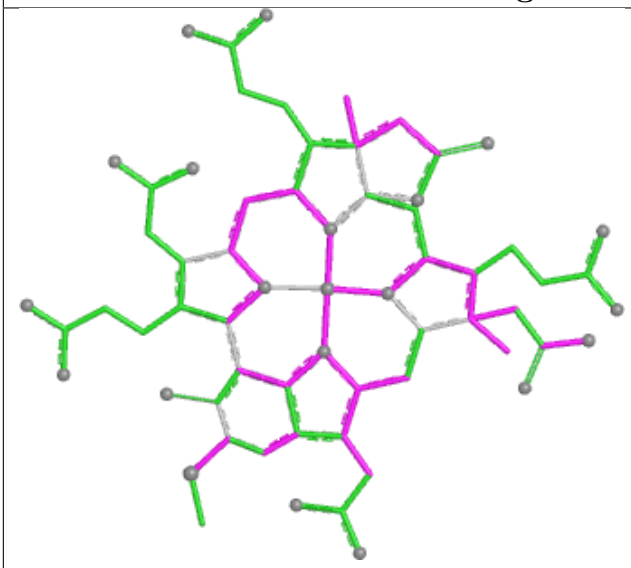
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	582	PGE	1	0
4	A	1002	TP7	1	0

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.

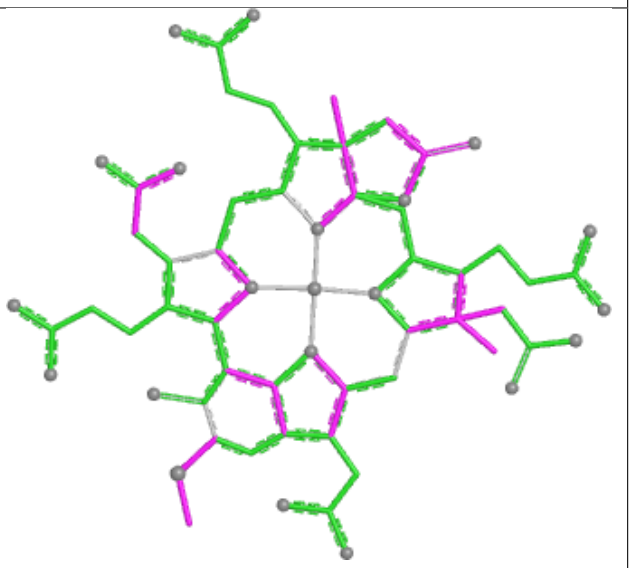
Ligand TP7 G 1002



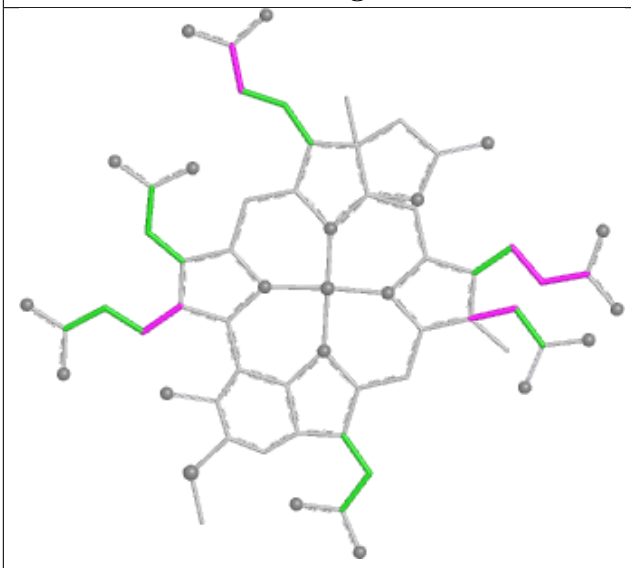
Ligand M43 G 1001



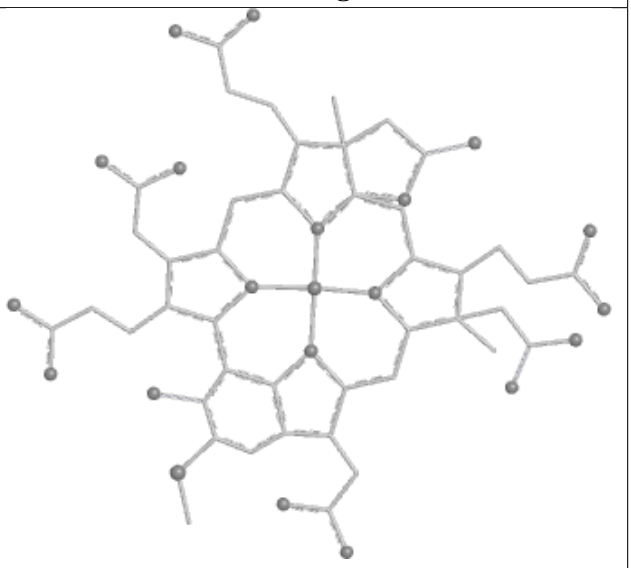
Bond lengths



Bond angles

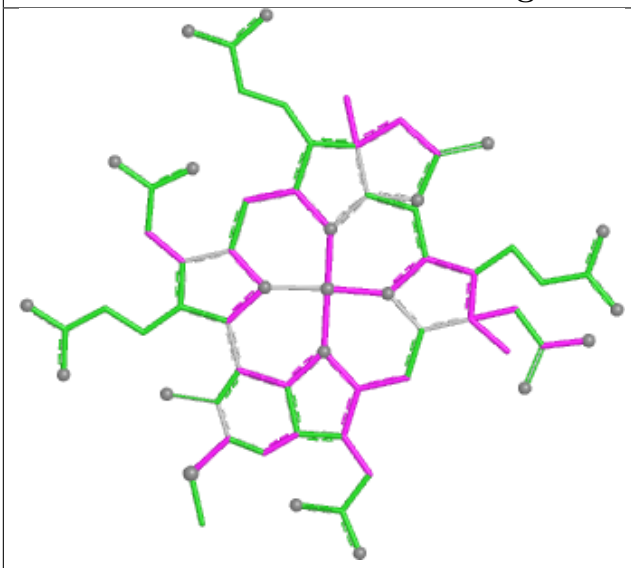


Torsions

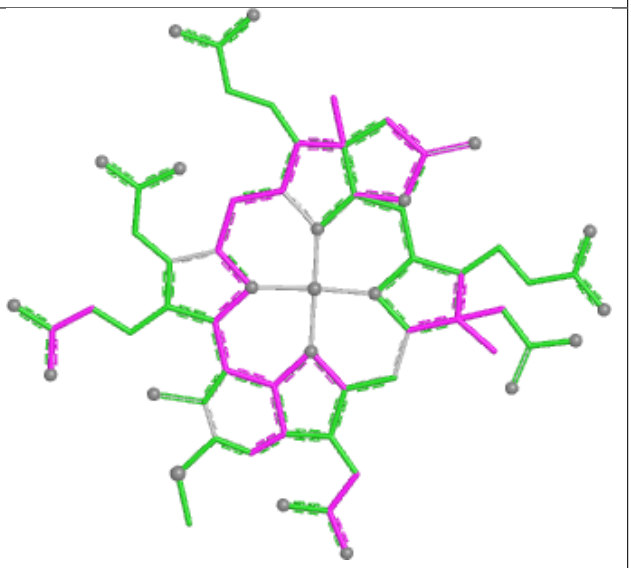


Rings

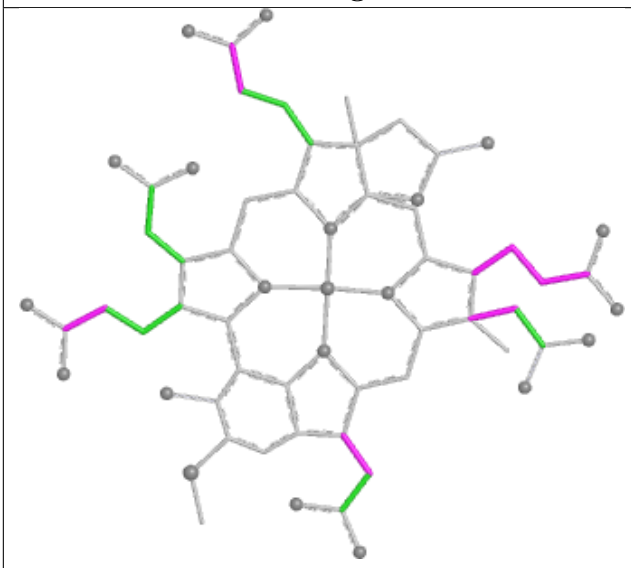
Ligand M43 A 1001



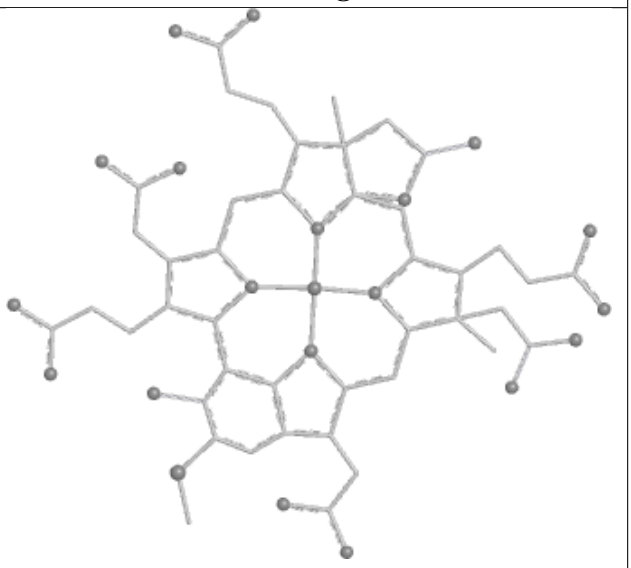
Bond lengths



Bond angles

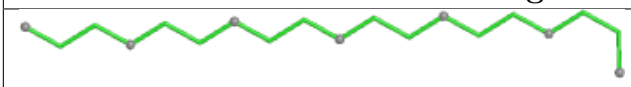


Torsions

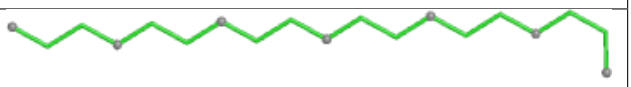


Rings

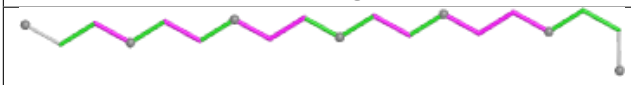
Ligand P6G B 434



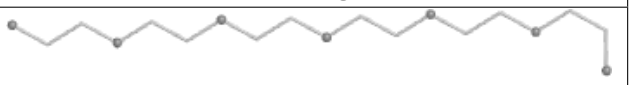
Bond lengths



Bond angles

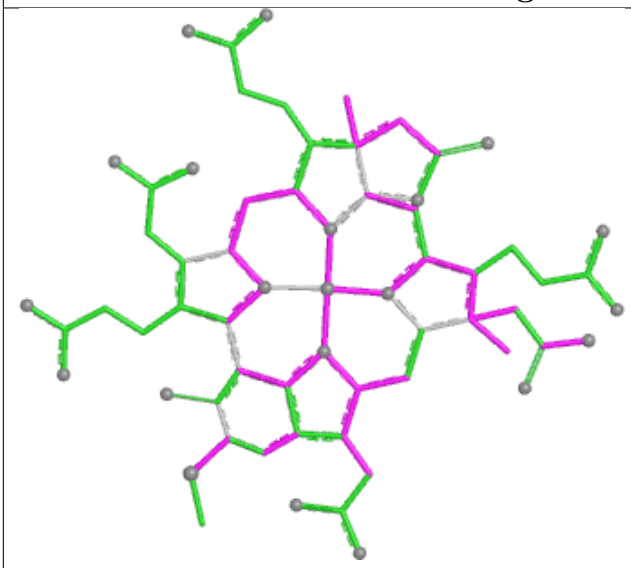


Torsions

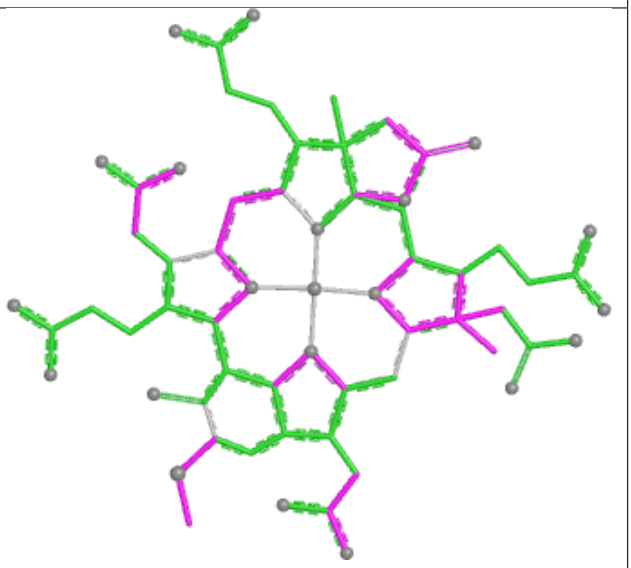


Rings

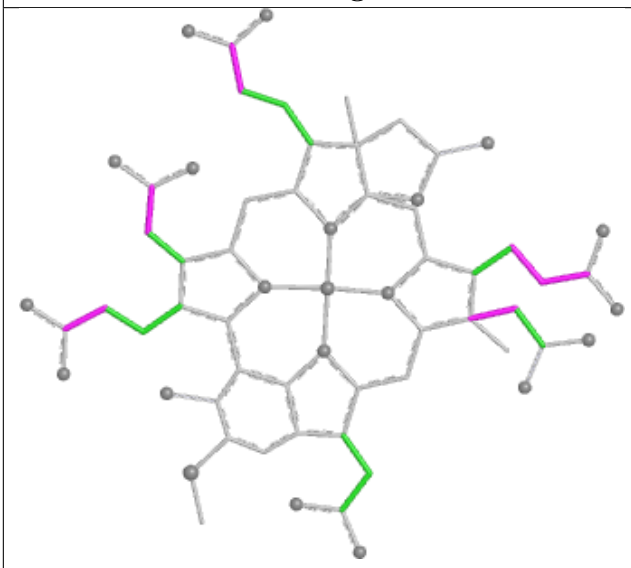
Ligand M43 D 1001



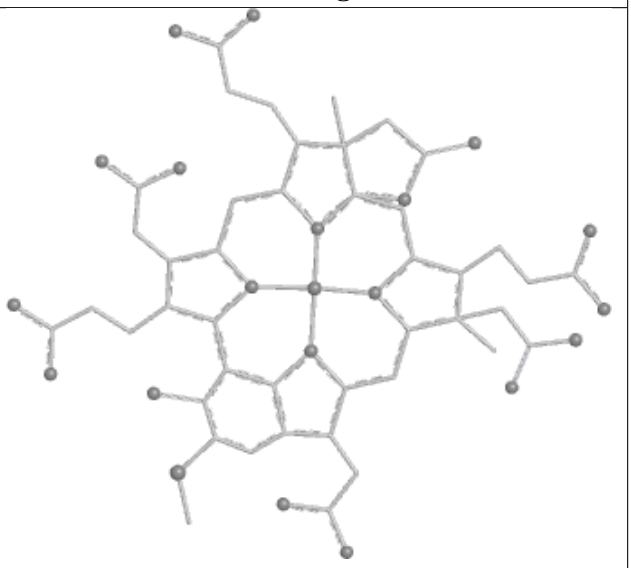
Bond lengths



Bond angles

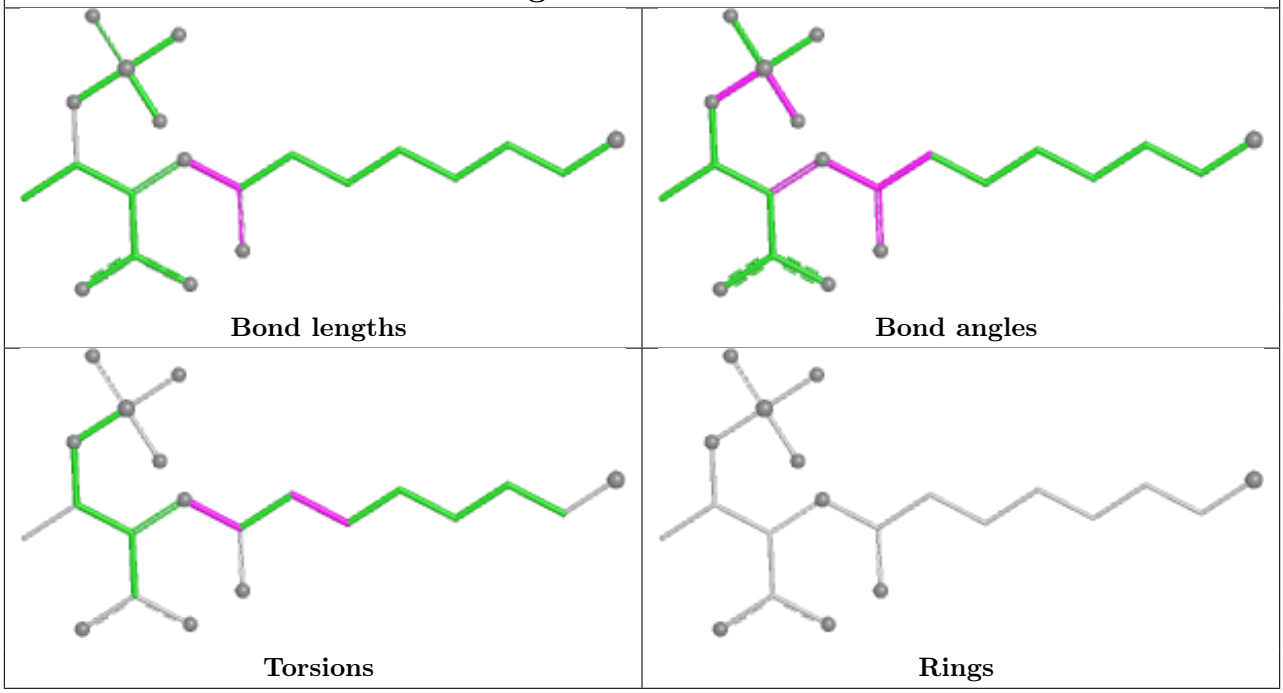


Torsions

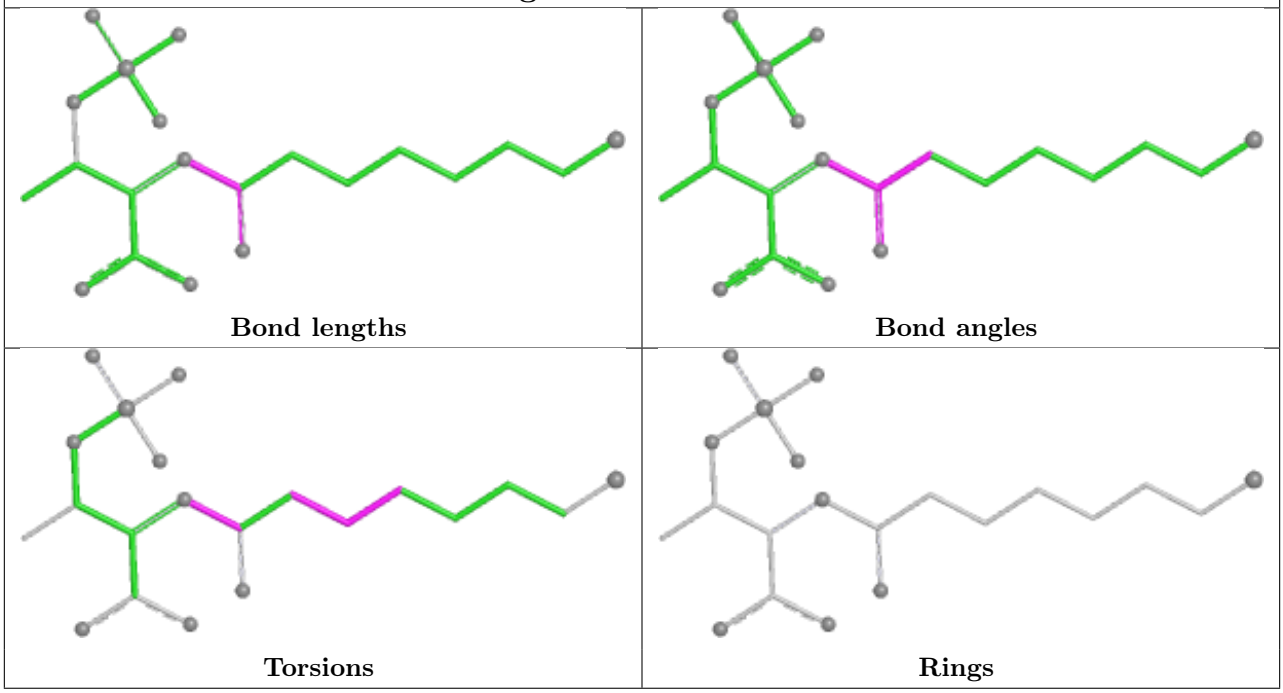


Rings

Ligand TP7 A 580



Ligand TP7 A 1002



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	574/579 (99%)	-0.74	0	100	100	16, 24, 36, 58	0
1	D	574/579 (99%)	-0.64	1 (0%)	91	92	17, 27, 40, 61	1 (0%)
1	G	574/579 (99%)	-0.61	1 (0%)	91	92	20, 28, 41, 68	0
2	B	431/433 (99%)	-0.25	1 (0%)	91	92	21, 37, 55, 79	0
2	E	431/433 (99%)	-0.02	2 (0%)	87	88	26, 42, 61, 83	0
2	H	431/433 (99%)	-0.09	0	100	100	26, 41, 58, 70	2 (0%)
3	C	278/279 (99%)	-0.41	0	100	100	20, 31, 48, 72	0
3	F	278/279 (99%)	-0.09	0	100	100	27, 42, 59, 96	1 (0%)
3	I	278/279 (99%)	-0.23	0	100	100	24, 38, 54, 96	0
All	All	3849/3873 (99%)	-0.39	5 (0%)	92	92	16, 33, 54, 96	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	579	LEU	2.9
2	E	76	VAL	2.7
2	B	75	ILE	2.5
2	E	433	LYS	2.1
1	D	579	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	MHS	G	271	11/12	0.95	0.07	30,32,34,34	0
1	MHS	D	271	11/12	0.97	0.05	24,26,27,27	0
1	0AF	D	333	15/16	0.97	0.05	19,22,24,26	0
1	MHO	D	499	9/10	0.97	0.07	23,29,30,30	0
1	MHS	A	271	11/12	0.97	0.06	28,29,32,32	0
1	0AF	G	333	15/16	0.97	0.05	21,25,26,27	0
1	MHO	G	499	9/10	0.97	0.06	21,26,31,32	0
1	0AF	A	333	15/16	0.98	0.05	17,22,23,24	0
1	MHO	A	499	9/10	0.98	0.05	18,22,24,24	0
1	GL3	A	464	4/5	0.99	0.04	21,22,24,24	0
1	GL3	G	464	4/5	0.99	0.04	27,28,28,29	0
1	GL3	D	464	4/5	0.99	0.05	29,32,32,34	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
9	SO4	A	585	5/5	0.72	0.10	110,110,110,110	0
13	GOL	C	281	6/6	0.76	0.16	37,44,45,46	0
7	1PE	F	281	16/16	0.77	0.17	56,63,68,68	0
8	PGE	D	582	10/10	0.79	0.17	58,62,68,69	0
9	SO4	D	584	5/5	0.85	0.11	98,98,99,99	0
7	1PE	D	580	16/16	0.86	0.16	42,61,62,63	0
9	SO4	H	435	5/5	0.86	0.10	65,66,67,68	5
5	COM	D	1003	7/7	0.86	0.22	17,23,45,46	7
9	SO4	C	282	5/5	0.87	0.12	62,63,63,66	0
9	SO4	I	281	5/5	0.87	0.11	64,64,65,67	5
9	SO4	B	435	5/5	0.87	0.09	63,64,64,65	5
9	SO4	B	436	5/5	0.88	0.14	71,72,72,73	5
9	SO4	A	584	5/5	0.88	0.14	53,54,56,58	5
8	PGE	G	582	10/10	0.89	0.12	49,51,57,58	0
7	1PE	H	434	16/16	0.89	0.12	43,47,51,52	0
5	COM	G	1003	7/7	0.89	0.16	17,28,33,35	7
9	SO4	D	583	5/5	0.89	0.10	85,85,86,86	0

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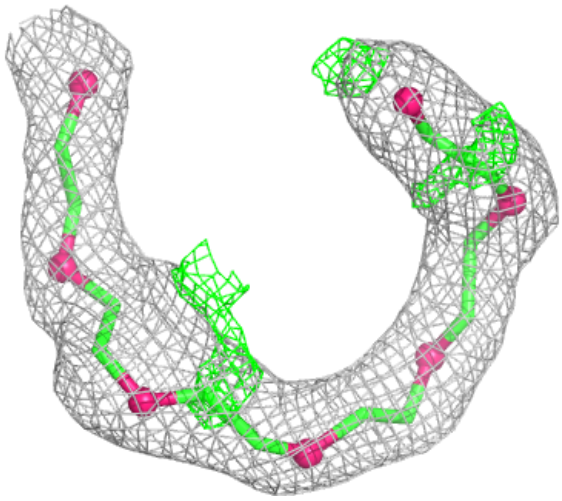
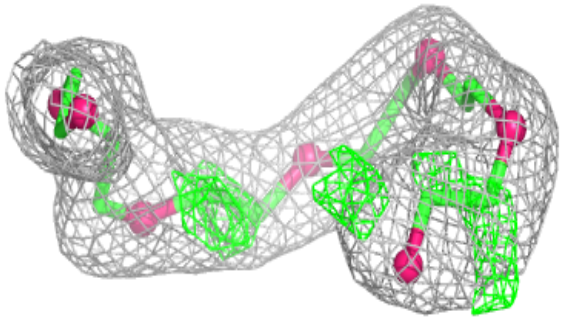
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	GOL	E	435	6/6	0.89	0.15	65,67,68,68	0
7	1PE	A	581	16/16	0.90	0.13	33,58,61,61	0
8	PGE	A	582	10/10	0.90	0.13	58,61,70,70	0
7	1PE	G	580	16/16	0.90	0.12	34,55,59,59	0
7	1PE	E	434	16/16	0.91	0.11	40,45,47,49	0
12	P6G	B	434	19/19	0.91	0.11	41,44,58,60	0
8	PGE	A	583	10/10	0.92	0.11	42,45,50,53	0
8	PGE	D	581	10/10	0.93	0.10	40,42,45,47	0
8	PGE	G	581	10/10	0.94	0.10	41,43,52,52	0
5	COM	A	1003	7/7	0.95	0.11	14,18,28,29	7
4	TP7	G	1002	21/21	0.97	0.06	21,26,33,37	0
4	TP7	A	580	21/21	0.98	0.06	24,29,30,31	0
6	M43	A	1001	64/64	0.98	0.06	20,28,33,36	0
6	M43	G	1001	64/64	0.98	0.06	16,26,31,33	0
11	CA	A	587	1/1	0.99	0.04	24,24,24,24	0
11	CA	G	583	1/1	0.99	0.07	22,22,22,22	1
4	TP7	A	1002	21/21	0.99	0.04	18,22,27,27	0
6	M43	D	1001	64/64	0.99	0.05	13,20,25,27	0
10	CL	A	586	1/1	0.99	0.16	47,47,47,47	0

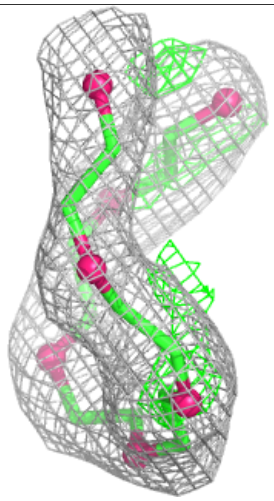
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G B 434:

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

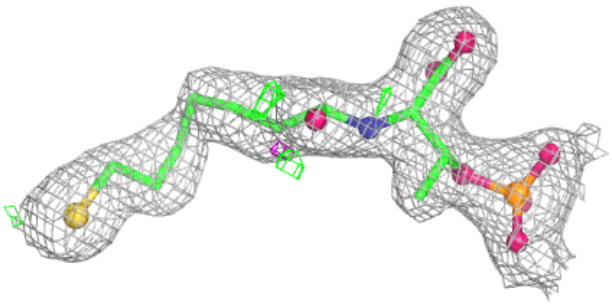


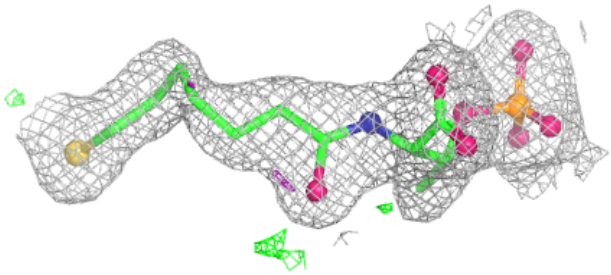


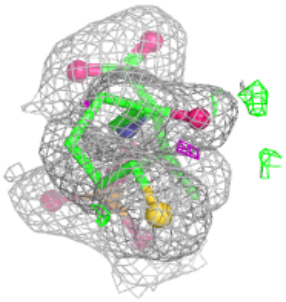


Electron density around TP7 G 1002:

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

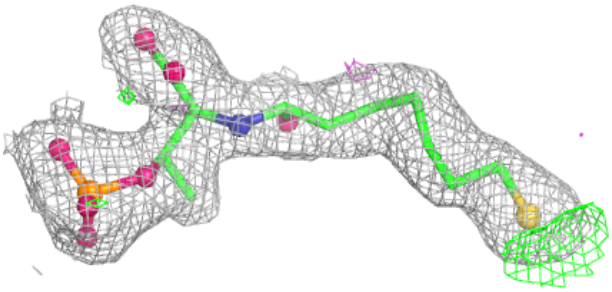


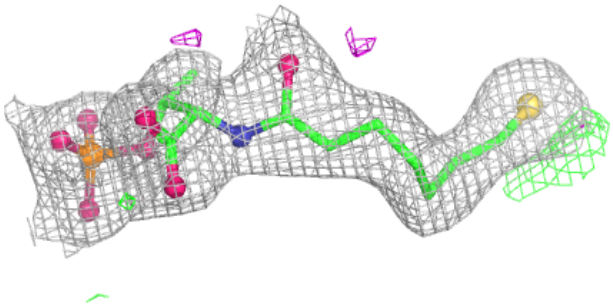


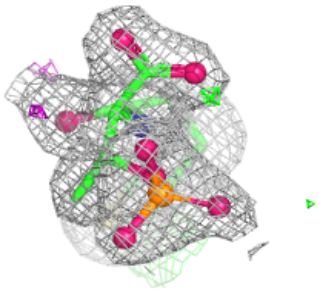


Electron density around TP7 A 580:

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

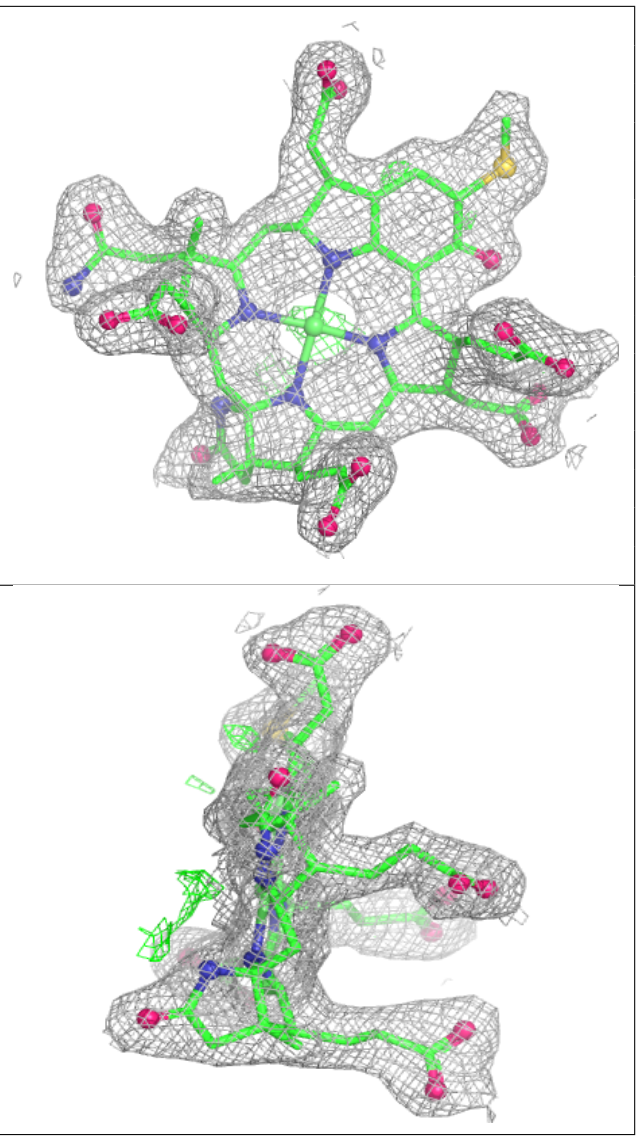






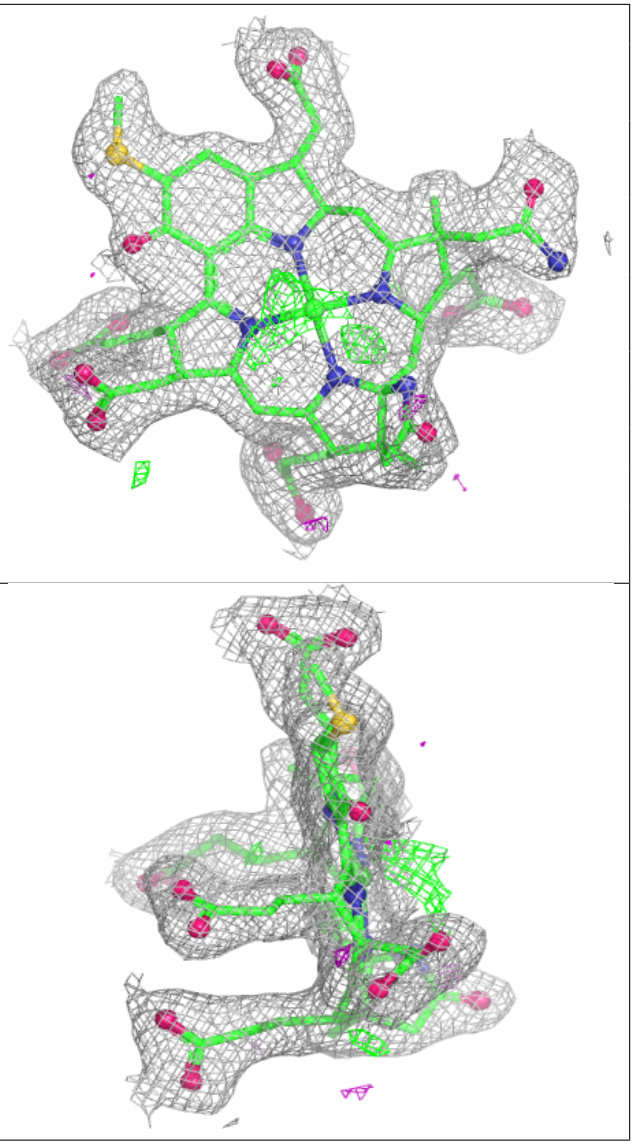
Electron density around M43 A 1001:

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



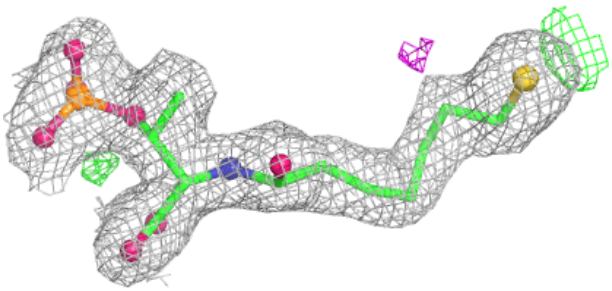
Electron density around M43 G 1001:

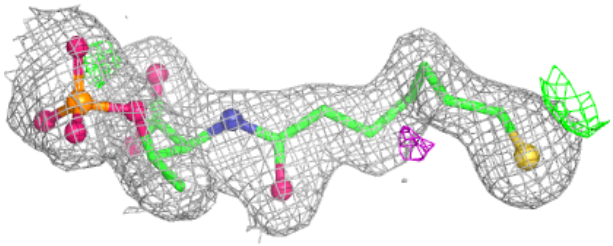
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

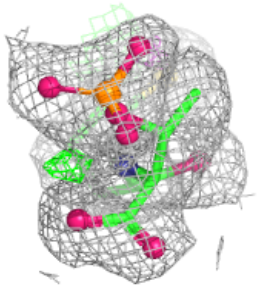


Electron density around TP7 A 1002:

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

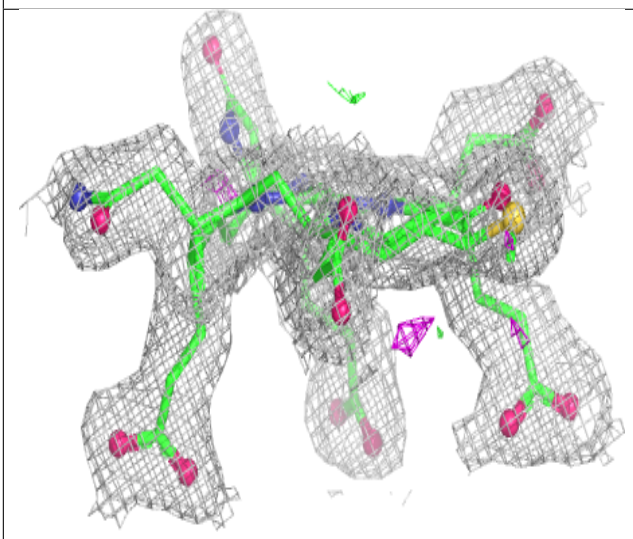


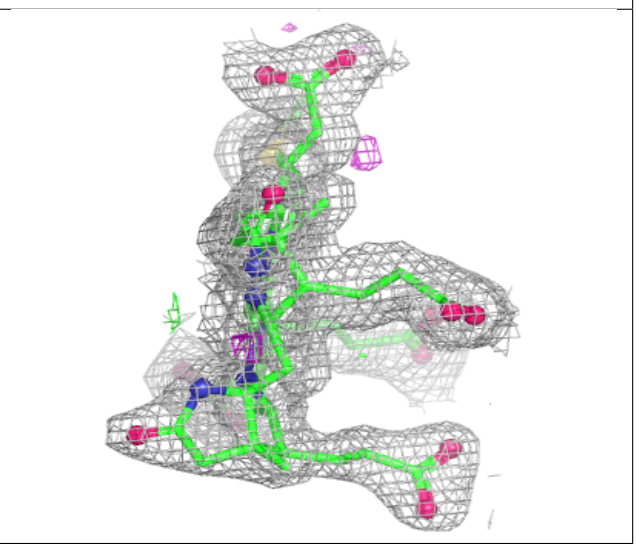




Electron density around M43 D 1001:

$2mF_o$-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.