Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2021 – 01:53 am BST

PDB ID	:	7NKG
Title	:	Methyl-coenzyme M reductase from Methermicoccus shengliensis at 1.6-A resolution
Authors	:	Mueller, M.; Wagner, T.
Deposited on	:	2021-02-18
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

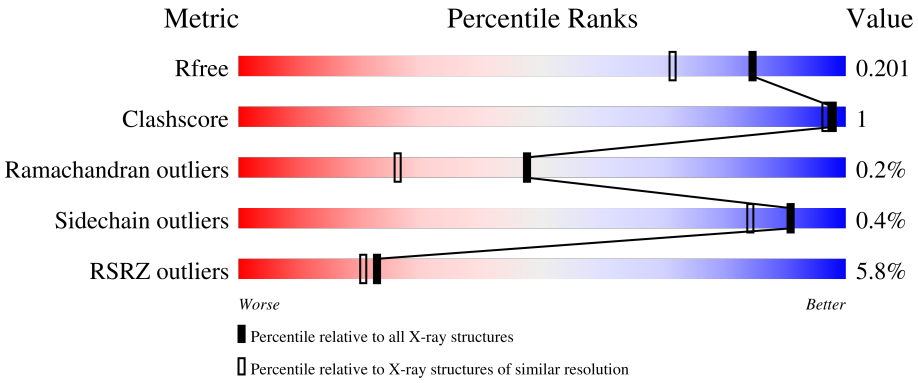
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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	569	96%
1	D	569	97%
1	G	569	14% 96%
1	J	569	6% 96%
2	B	433	99%

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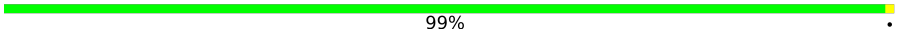
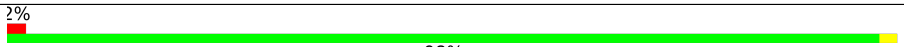
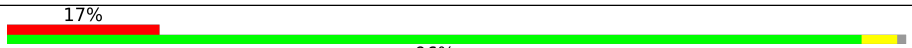
Mol	Chain	Length	Quality of chain
2	E	433	
2	H	433	
2	K	433	
3	C	248	
3	F	248	
3	I	248	
3	L	248	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 42790 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
1	A	564	Total	C	N	O	S	0	5	0
			4368	2769	737	841	21			
1	D	565	Total	C	N	O	S	0	4	0
			4380	2776	742	841	21			
1	G	562	Total	C	N	O	S	0	1	0
			4325	2744	731	829	21			
1	J	563	Total	C	N	O	S	0	0	0
			4332	2746	735	830	21			

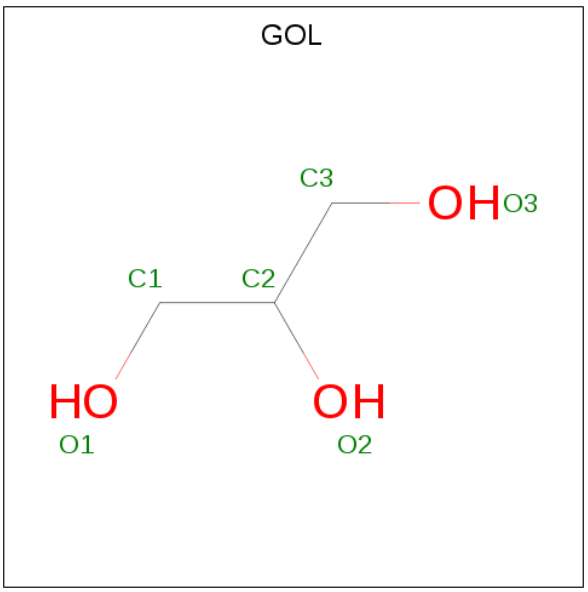
- Molecule 2 is a protein called Methyl-coenzyme M reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	1	0
			3215	2022	555	621	17			
2	E	432	Total	C	N	O	S	0	3	0
			3230	2034	555	624	17			
2	H	432	Total	C	N	O	S	0	2	0
			3224	2027	556	624	17			
2	K	432	Total	C	N	O	S	0	0	0
			3209	2019	555	618	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	3	0
			1981	1228	361	379	13			
3	F	247	Total	C	N	O	S	0	1	0
			1968	1220	357	378	13			
3	I	238	Total	C	N	O	S	0	0	0
			1898	1175	346	366	11			
3	L	246	Total	C	N	O	S	0	0	0
			1957	1213	356	376	12			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

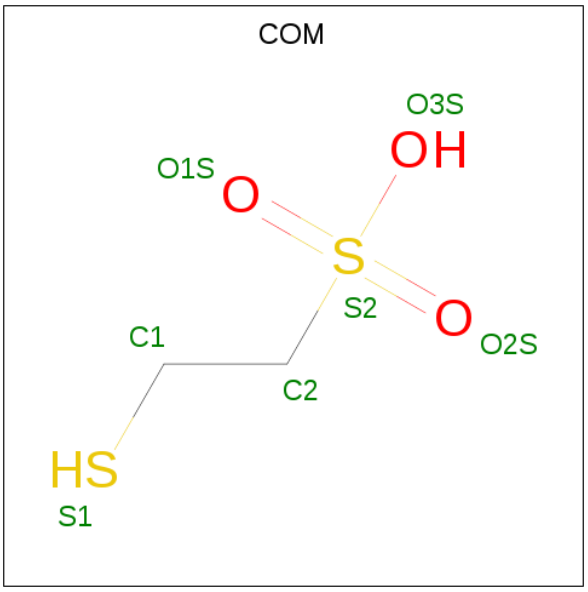


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

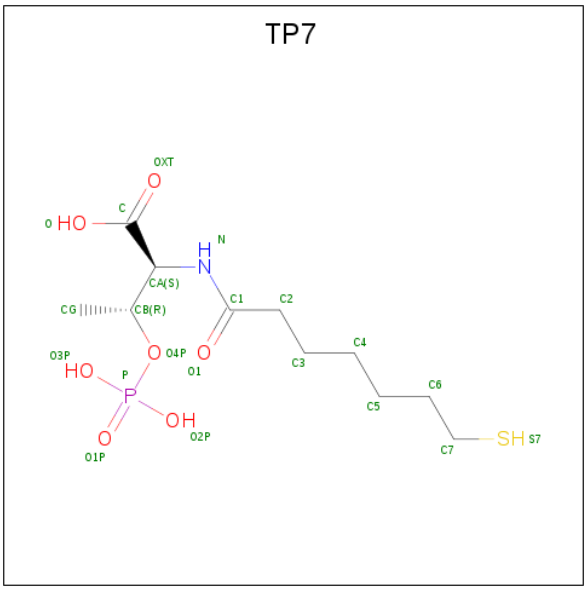
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



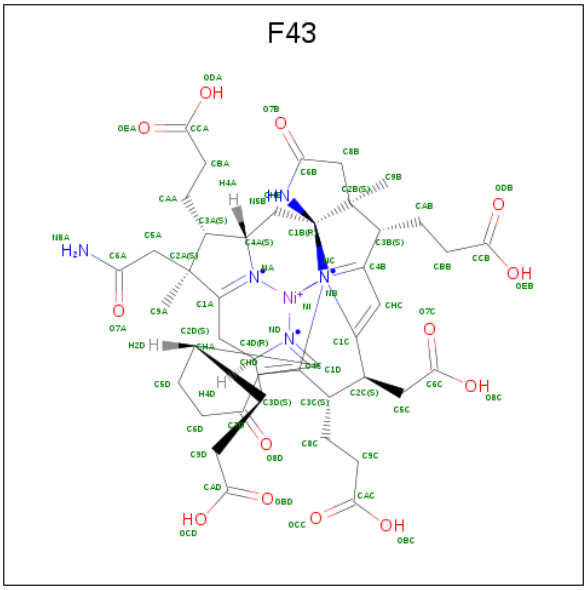
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O S 7 2 3 2	0	0
6	D	1	Total C O S 7 2 3 2	0	0
6	G	1	Total C O S 7 2 3 2	0	0
6	J	1	Total C O S 7 2 3 2	0	0

- Molecule 7 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



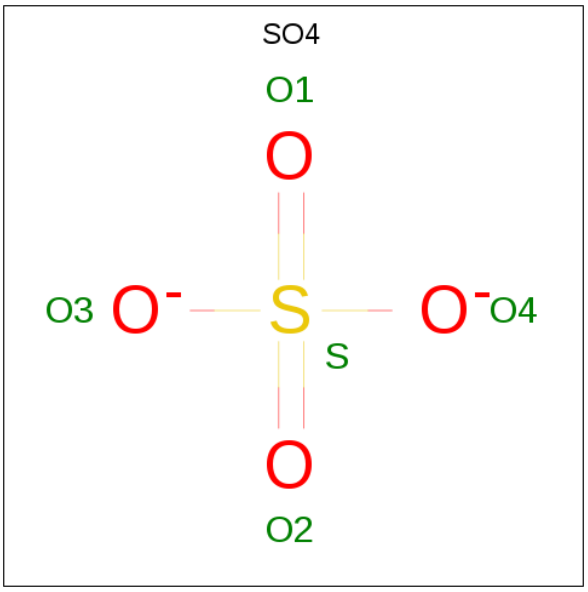
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
7	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
7	G	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
7	G	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 8 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
8	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
8	G	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
8	J	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0
9	H	1	Total O S 5 4 1	0	0
9	K	1	Total O S 5 4 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	641	Total O 641 641	0	1
10	B	409	Total O 409 409	0	1
10	C	321	Total O 321 321	0	3
10	D	617	Total O 617 617	0	6
10	E	475	Total O 475 475	0	0
10	F	303	Total O 303 303	0	0
10	G	315	Total O 315 315	0	1

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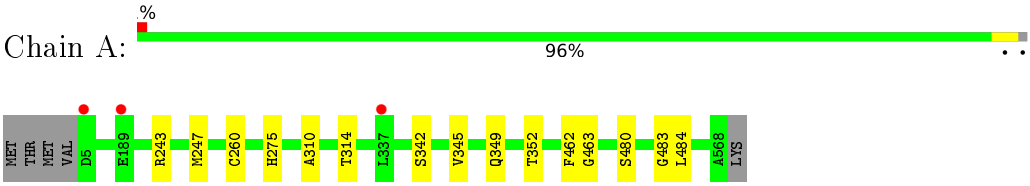
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	258	Total O 258 258	0	0
10	I	159	Total O 159 159	0	0
10	J	424	Total O 424 424	0	1
10	K	223	Total O 223 223	0	0
10	L	153	Total O 153 153	0	0

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.

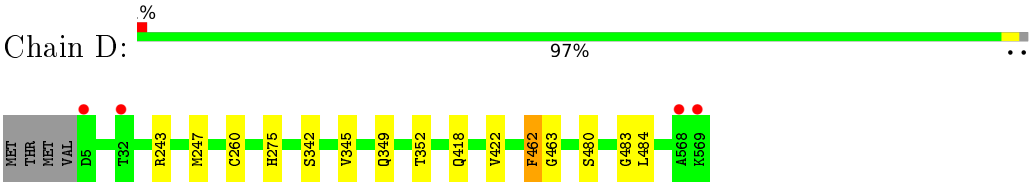
- Molecule 1: Methyl-coenzyme M reductase alpha subunit

Chain A:



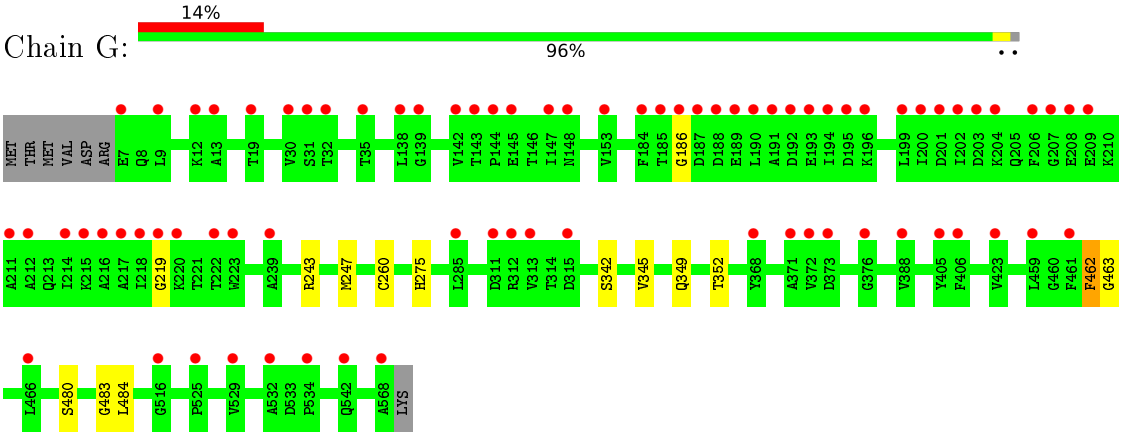
- Molecule 1: Methyl-coenzyme M reductase alpha subunit

Chain D:



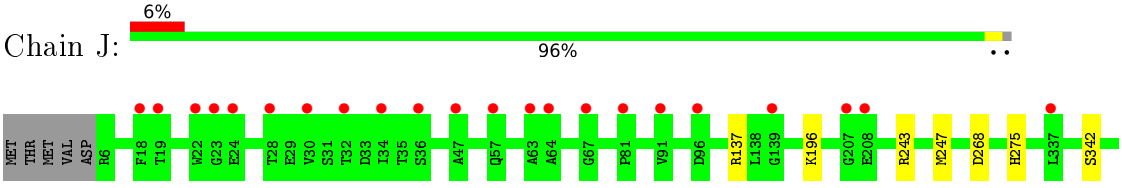
- Molecule 1: Methyl-coenzyme M reductase alpha subunit

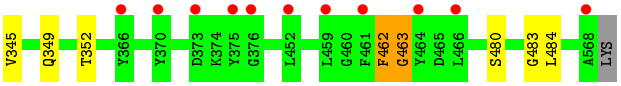
Chain G:



- Molecule 1: Methyl-coenzyme M reductase alpha subunit

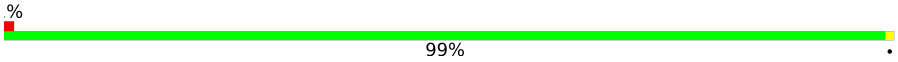
Chain J:

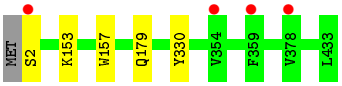




• Molecule 2: Methyl-coenzyme M reductase beta subunit

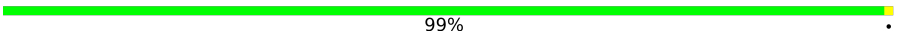
Chain B:

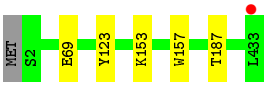




• Molecule 2: Methyl-coenzyme M reductase beta subunit

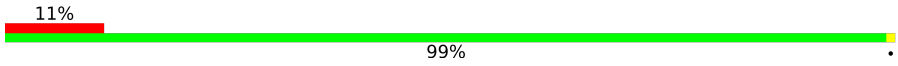
Chain E:

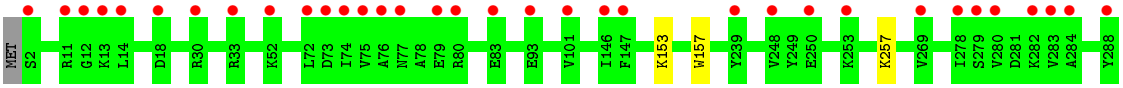


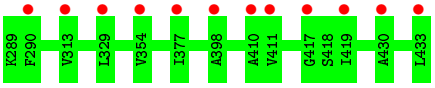


• Molecule 2: Methyl-coenzyme M reductase beta subunit

Chain H:

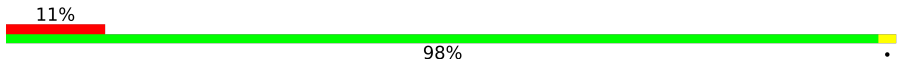


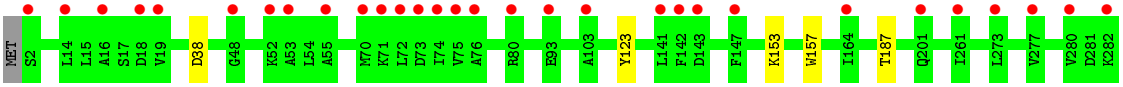


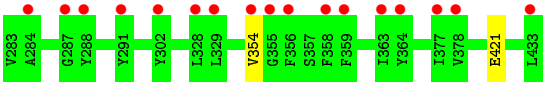


• Molecule 2: Methyl-coenzyme M reductase beta subunit

Chain K:

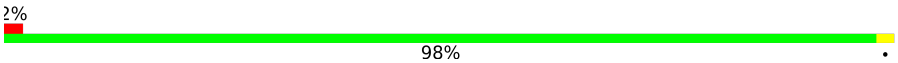


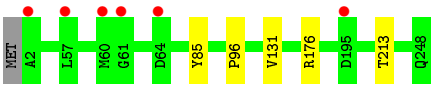




• Molecule 3: Methyl-coenzyme M reductase gamma subunit

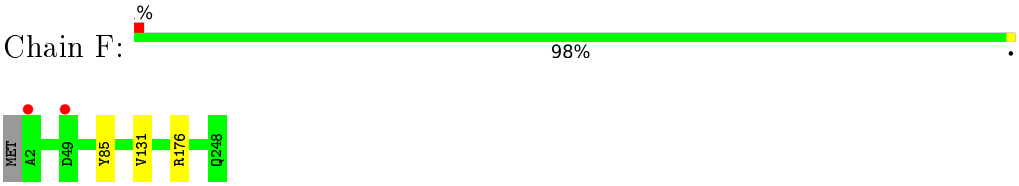
Chain C:





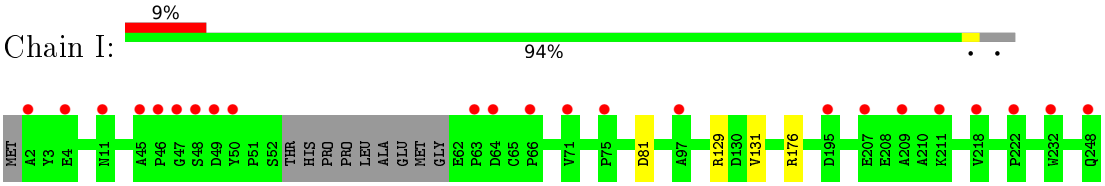
• Molecule 3: Methyl-coenzyme M reductase gamma subunit

Chain F:



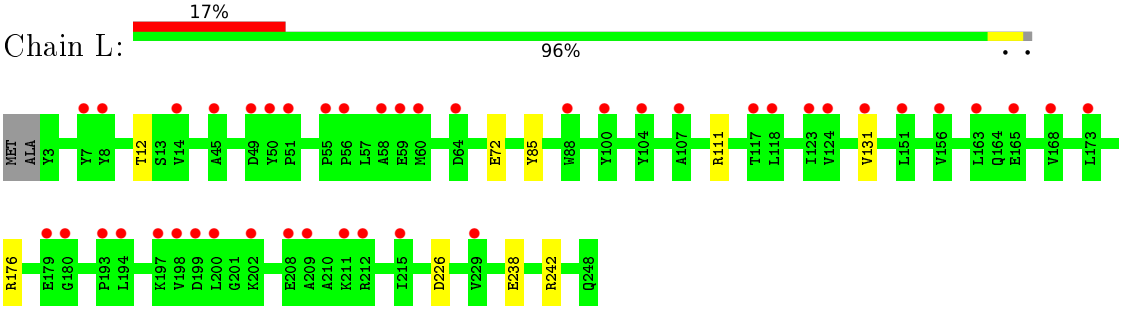
• Molecule 3: Methyl-coenzyme M reductase gamma subunit

Chain I:



• Molecule 3: Methyl-coenzyme M reductase gamma subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.62Å 148.18Å 235.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 1.60 48.36 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.36-1.60) 99.7 (48.36-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.60Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.172 , 0.190 0.182 , 0.201	Depositor DCC
R_{free} test set	30001 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	42790	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: SO4, GL3, F43, K, AGM, TP7, GOL, COM, MHS

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	0.42	0/4441	0.57	0/6017
1	D	0.41	0/4444	0.57	0/6019
1	G	0.36	0/4389	0.57	0/5948
1	J	0.38	0/4393	0.57	0/5952
2	B	0.40	0/3267	0.56	0/4421
2	E	0.41	0/3289	0.56	0/4451
2	H	0.37	0/3276	0.56	0/4433
2	K	0.37	0/3258	0.56	0/4410
3	C	0.41	0/2036	0.60	0/2759
3	F	0.42	0/2017	0.60	0/2734
3	I	0.37	0/1940	0.59	0/2627
3	L	0.38	0/2003	0.60	0/2717
All	All	0.39	0/38753	0.57	0/52488

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	330	TYR	Sidechain

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	4368	0	4258	6	0
1	D	4380	0	4271	9	0
1	G	4325	0	4219	8	0
1	J	4332	0	4223	8	0
2	B	3215	0	3228	2	0
2	E	3230	0	3243	3	0
2	H	3224	0	3233	1	0
2	K	3209	0	3224	4	0
3	C	1981	0	1921	3	0
3	F	1968	0	1902	1	0
3	I	1898	0	1830	1	0
3	L	1957	0	1888	5	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	E	6	0	8	0	0
5	A	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	5	0	0
6	D	7	0	5	2	0
6	G	7	0	5	3	0
6	J	7	0	5	3	0
7	A	42	0	38	1	0
7	G	42	0	38	0	0
8	A	62	0	43	2	0
8	D	62	0	43	1	0
8	G	62	0	43	4	0
8	J	62	0	43	3	0
9	B	5	0	0	0	0
9	E	10	0	0	1	0
9	H	5	0	0	0	0
9	K	5	0	0	0	0
10	A	641	0	0	0	0
10	B	409	0	0	1	0
10	C	321	0	0	0	0
10	D	617	0	0	0	0
10	E	475	0	0	0	0
10	F	303	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	G	315	0	0	0	0
10	H	258	0	0	0	0
10	I	159	0	0	0	0
10	J	424	0	0	1	0
10	K	223	0	0	0	0
10	L	153	0	0	0	0
All	All	42790	0	37732	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (51) 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)
8:G:605:F43:H9A1	1:J:345:VAL:HB	1.88	0.55
1:G:345:VAL:HB	8:J:602:F43:H9A1	1.86	0.55
3:L:12:THR:HG23	3:L:226:ASP:CG	2.26	0.55
1:A:345:VAL:HB	8:D:602:F43:H9A1	1.89	0.54
3:L:72:GLU:O	3:L:111:ARG:NH2	2.41	0.53
8:A:606:F43:H9A1	1:D:345:VAL:HB	1.90	0.53
7:A:604:TP7:O1P	1:D:275:MHS:NE2	2.43	0.52
3:C:85:TYR:CE1	1:D:260:CYS:HB2	2.47	0.50
3:L:238:GLU:OE2	3:L:242:ARG:NH1	2.45	0.50
1:G:349:GLN:HA	1:G:352:THR:OG1	2.13	0.48
1:J:349:GLN:HA	1:J:352:THR:OG1	2.13	0.48
1:D:349:GLN:HA	1:D:352:THR:OG1	2.14	0.48
1:D:418:GLN:O	1:D:422[B]:VAL:HG12	2.13	0.48
1:A:260:CYS:HB2	3:F:85:TYR:CE1	2.48	0.48
2:E:69:GLU:OE1	9:E:501:SO4:O4	2.31	0.48
2:H:153:LYS:HD2	2:H:157:TRP:CD1	2.49	0.48
1:A:349:GLN:HA	1:A:352:THR:OG1	2.13	0.47
2:E:123[A]:TYR:CE1	2:E:187:THR:HG21	2.49	0.47
2:K:123:TYR:CE1	2:K:187:THR:HG21	2.50	0.46
3:C:96:PRO:HA	3:C:213:THR:HA	1.97	0.46
8:G:605:F43:N5B	6:J:601:COM:H22	2.31	0.46
1:J:196:LYS:NZ	10:J:705:HOH:O	2.48	0.45
8:A:606:F43:C1C	6:D:601:COM:H12	2.47	0.45
1:D:462:PHE:HB2	6:D:601:COM:O3S	2.17	0.45
1:J:462:PHE:HB2	6:J:601:COM:O2S	2.16	0.45
2:K:153:LYS:HD2	2:K:157:TRP:CD1	2.52	0.44
1:D:483:GLY:O	1:D:484:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:O	1:A:247:MET:HG2	2.19	0.43
1:D:243:ARG:O	1:D:247:MET:HG2	2.18	0.43
1:G:462:PHE:HB2	6:G:602:COM:O1S	2.19	0.43
1:G:483:GLY:O	1:G:484:LEU:HB2	2.18	0.43
1:G:260:CYS:HB2	3:L:85:TYR:CE1	2.54	0.43
1:J:483:GLY:O	1:J:484:LEU:HB2	2.18	0.43
1:G:243:ARG:O	1:G:247:MET:HG2	2.19	0.42
1:J:243:ARG:O	1:J:247:MET:HG2	2.19	0.42
1:J:463:GL3:HA2	2:K:354:VAL:HG12	2.01	0.42
1:G:186:GLY:HA3	1:G:219:GLY:O	2.19	0.42
3:I:81:ASP:OD2	3:I:129:ARG:HG3	2.19	0.42
3:C:85:TYR:CZ	1:D:260:CYS:HB2	2.55	0.42
8:G:605:F43:H3C	8:G:605:F43:O8D	2.20	0.41
8:G:605:F43:C6B	6:J:601:COM:H22	2.50	0.41
1:A:483:GLY:O	1:A:484:LEU:HB2	2.20	0.41
6:G:602:COM:H12	8:J:602:F43:C1C	2.51	0.41
2:B:179:GLN:HB3	10:B:889:HOH:O	2.21	0.41
1:G:260:CYS:HB2	3:L:85:TYR:CZ	2.56	0.41
2:B:153:LYS:HD2	2:B:157:TRP:CD1	2.56	0.41
6:G:602:COM:H12	8:J:602:F43:CHC	2.51	0.40
1:J:137:ARG:NH2	1:J:268:ASP:OD2	2.53	0.40
2:E:153:LYS:HD2	2:E:157:TRP:CD1	2.55	0.40
2:K:38:ASP:OD2	2:K:421:GLU:OE2	2.39	0.40
1:A:310:ALA:O	1:A:314:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	564/569 (99%)	545 (97%)	17 (3%)	2 (0%)	34 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	564/569 (99%)	546 (97%)	16 (3%)	2 (0%)	34 15
1	G	558/569 (98%)	539 (97%)	17 (3%)	2 (0%)	34 15
1	J	558/569 (98%)	539 (97%)	17 (3%)	2 (0%)	34 15
2	B	431/433 (100%)	427 (99%)	4 (1%)	0	100 100
2	E	433/433 (100%)	427 (99%)	6 (1%)	0	100 100
2	H	432/433 (100%)	427 (99%)	5 (1%)	0	100 100
2	K	430/433 (99%)	425 (99%)	5 (1%)	0	100 100
3	C	248/248 (100%)	244 (98%)	4 (2%)	0	100 100
3	F	246/248 (99%)	242 (98%)	4 (2%)	0	100 100
3	I	234/248 (94%)	230 (98%)	4 (2%)	0	100 100
3	L	244/248 (98%)	238 (98%)	6 (2%)	0	100 100
All	All	4942/5000 (99%)	4829 (98%)	105 (2%)	8 (0%)	47 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	SER
1	A	480	SER
1	D	342	SER
1	D	480	SER
1	G	342	SER
1	G	480	SER
1	J	342	SER
1	J	480	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	440/440 (100%)	439 (100%)	1 (0%)	93 88
1	D	440/440 (100%)	439 (100%)	1 (0%)	93 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	434/440 (99%)	433 (100%)	1 (0%)	93 88
1	J	434/440 (99%)	433 (100%)	1 (0%)	93 88
2	B	335/335 (100%)	334 (100%)	1 (0%)	92 87
2	E	337/335 (101%)	337 (100%)	0	100 100
2	H	336/335 (100%)	335 (100%)	1 (0%)	92 87
2	K	334/335 (100%)	334 (100%)	0	100 100
3	C	212/210 (101%)	210 (99%)	2 (1%)	78 65
3	F	210/210 (100%)	208 (99%)	2 (1%)	76 61
3	I	202/210 (96%)	200 (99%)	2 (1%)	76 61
3	L	209/210 (100%)	207 (99%)	2 (1%)	76 61
All	All	3923/3940 (100%)	3909 (100%)	14 (0%)	91 84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	PHE
2	B	2	SER
3	C	131	VAL
3	C	176	ARG
1	D	462	PHE
3	F	131	VAL
3	F	176	ARG
1	G	462	PHE
2	H	257	LYS
3	I	131	VAL
3	I	176	ARG
1	J	462	PHE
3	L	131	VAL
3	L	176	ARG

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

5.3.3 RNA

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	AGM	D	289	1	10,11,12	0.35	0	6,13,15	0.25	0
1	AGM	J	289	1	10,11,12	0.34	0	6,13,15	0.25	0
1	MHS	J	275	1	7,11,12	0.56	0	6,14,16	1.32	1 (16%)
1	GL3	D	463	1	2,3,4	3.68	1 (50%)	1,2,4	0.25	0
1	GL3	G	463	1	2,3,4	3.45	1 (50%)	1,2,4	0.28	0
1	MHS	G	275	1	7,11,12	0.52	0	6,14,16	1.32	1 (16%)
1	GL3	A	463	1	2,3,4	3.31	1 (50%)	1,2,4	0.20	0
1	GL3	J	463	1	2,3,4	3.31	1 (50%)	1,2,4	0.15	0
1	MHS	A	275	1	7,11,12	0.58	0	6,14,16	1.32	1 (16%)
1	MHS	D	275	1	7,11,12	0.68	0	6,14,16	1.33	0
1	AGM	A	289	1	10,11,12	0.33	0	6,13,15	0.30	0
1	AGM	G	289	1	10,11,12	0.32	0	6,13,15	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	D	289	1	-	0/10/11/13	-
1	AGM	J	289	1	-	0/10/11/13	-
1	MHS	J	275	1	-	0/5/6/8	0/1/1/1
1	GL3	D	463	1	-	1/1/1/2	-
1	GL3	G	463	1	-	1/1/1/2	-
1	MHS	G	275	1	-	0/5/6/8	0/1/1/1
1	GL3	A	463	1	-	0/1/1/2	-
1	GL3	J	463	1	-	1/1/1/2	-
1	MHS	A	275	1	-	0/5/6/8	0/1/1/1
1	MHS	D	275	1	-	0/5/6/8	0/1/1/1
1	AGM	A	289	1	-	0/10/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	G	289	1	-	0/10/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	463	GL3	C-S	-5.20	1.62	1.80
1	G	463	GL3	C-S	-4.88	1.63	1.80
1	A	463	GL3	C-S	-4.68	1.64	1.80
1	J	463	GL3	C-S	-4.68	1.64	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	275	MHS	NE2-CE1-ND1	-2.30	108.85	112.26
1	A	275	MHS	NE2-CE1-ND1	-2.29	108.86	112.26
1	G	275	MHS	NE2-CE1-ND1	-2.26	108.91	112.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	463	GL3	S-C-CA-N
1	G	463	GL3	S-C-CA-N
1	D	463	GL3	S-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	463	GL3	1	0
1	D	275	MHS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
8	F43	G	605	6,1	46,71,71	2.38	7 (15%)	48,118,118	1.47	12 (25%)
7	TP7	A	605	-	16,20,20	0.64	0	18,26,26	0.66	0
8	F43	J	602	6,1	46,71,71	2.35	6 (13%)	48,118,118	1.41	9 (18%)
9	SO4	E	503	-	4,4,4	0.39	0	6,6,6	0.21	0
7	TP7	G	604	-	16,20,20	0.62	0	18,26,26	0.80	0
4	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.30	0
9	SO4	E	501	-	4,4,4	0.35	0	6,6,6	0.16	0
9	SO4	K	501	-	4,4,4	0.36	0	6,6,6	0.05	0
9	SO4	H	501	-	4,4,4	0.34	0	6,6,6	0.07	0
9	SO4	B	501	-	4,4,4	0.35	0	6,6,6	0.14	0
4	GOL	A	601	-	5,5,5	0.26	0	5,5,5	0.26	0
6	COM	A	603	8	6,6,6	1.29	0	7,8,8	1.67	2 (28%)
8	F43	A	606	6,1	46,71,71	2.46	6 (13%)	48,118,118	1.38	7 (14%)
4	GOL	E	502	-	5,5,5	0.27	0	5,5,5	0.34	0
6	COM	G	602	8	6,6,6	1.50	2 (33%)	7,8,8	2.29	2 (28%)
6	COM	J	601	8	6,6,6	1.44	2 (33%)	7,8,8	2.43	4 (57%)
7	TP7	G	603	-	16,20,20	0.67	0	18,26,26	0.72	0
8	F43	D	602	6,1	46,71,71	2.42	6 (13%)	48,118,118	1.44	8 (16%)
7	TP7	A	604	-	16,20,20	0.54	0	18,26,26	0.69	0
6	COM	D	601	8	6,6,6	1.41	2 (33%)	7,8,8	2.23	3 (42%)

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	GOL	B	502	-	-	0/4/4/4	-
8	F43	G	605	6,1	-	1/18/185/185	-
7	TP7	A	604	-	-	1/20/24/24	-
7	TP7	A	605	-	-	0/20/24/24	-
8	F43	J	602	6,1	-	1/18/185/185	-
6	COM	G	602	8	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	COM	J	601	8	-	0/4/4/4	-
8	F43	A	606	6,1	-	2/18/185/185	-
7	TP7	G	603	-	-	1/20/24/24	-
8	F43	D	602	6,1	-	1/18/185/185	-
4	GOL	A	601	-	-	2/4/4/4	-
6	COM	D	601	8	-	0/4/4/4	-
6	COM	A	603	8	-	0/4/4/4	-
4	GOL	E	502	-	-	0/4/4/4	-
7	TP7	G	604	-	-	1/20/24/24	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	602	F43	NI-NA	8.98	2.08	1.89
8	A	606	F43	NI-NA	8.76	2.08	1.89
8	D	602	F43	NI-NA	8.67	2.08	1.89
8	A	606	F43	NI-NB	8.30	2.07	1.89
8	D	602	F43	NI-NB	8.27	2.07	1.89
8	G	605	F43	NI-NB	8.03	2.06	1.89
8	A	606	F43	NI-ND	7.58	2.05	1.89
8	D	602	F43	NI-ND	7.42	2.05	1.89
8	G	605	F43	NI-ND	7.31	2.05	1.89
8	G	605	F43	NI-NA	7.28	2.05	1.89
8	J	602	F43	NI-NB	7.25	2.05	1.89
8	J	602	F43	NI-ND	7.02	2.04	1.89
8	G	605	F43	CHD-C1D	-6.59	1.34	1.43
8	A	606	F43	CHD-C1D	-5.98	1.35	1.43
8	D	602	F43	CHD-C1D	-5.77	1.35	1.43
8	J	602	F43	CHD-C1D	-5.74	1.35	1.43
8	D	602	F43	CHC-C4B	3.24	1.48	1.39
8	G	605	F43	C4D-ND	-2.94	1.44	1.49
8	J	602	F43	CHC-C4B	2.94	1.47	1.39
8	A	606	F43	CHC-C4B	2.93	1.47	1.39
8	G	605	F43	CHC-C4B	2.78	1.47	1.39
6	G	602	COM	O2S-S2	2.77	1.53	1.45
6	J	601	COM	O2S-S2	2.37	1.52	1.45
8	A	606	F43	CHD-C7D	2.24	1.51	1.46
6	D	601	COM	O2S-S2	2.22	1.51	1.45
6	D	601	COM	O1S-S2	2.18	1.51	1.45
8	D	602	F43	CHD-C7D	2.12	1.50	1.46
6	J	601	COM	O1S-S2	2.12	1.51	1.45
8	G	605	F43	C4A-NA	-2.11	1.46	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	602	COM	O1S-S2	2.04	1.51	1.45
8	J	602	F43	CHD-C7D	2.02	1.50	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	601	COM	O2S-S2-C2	4.49	112.32	106.92
6	G	602	COM	O3S-S2-C2	4.45	112.97	105.77
8	A	606	F43	O8D-C7D-C6D	-4.16	114.04	120.86
6	J	601	COM	O3S-S2-C2	3.82	111.94	105.77
8	D	602	F43	O8D-C7D-C6D	-3.72	114.76	120.86
8	G	605	F43	C9A-C2A-C3A	3.36	117.94	112.98
6	J	601	COM	O2S-S2-O1S	-3.35	102.36	113.95
8	J	602	F43	O8D-C7D-C6D	-3.30	115.46	120.86
6	A	603	COM	O2S-S2-C2	3.23	110.81	106.92
8	J	602	F43	C9A-C2A-C3A	3.19	117.68	112.98
6	G	602	COM	O3S-S2-O2S	-3.10	103.69	111.27
8	D	602	F43	C6D-C7D-CHD	3.01	122.60	116.95
6	J	601	COM	O1S-S2-C2	2.90	110.41	106.92
8	G	605	F43	C9D-C3D-C4D	-2.89	107.05	114.67
8	G	605	F43	O7B-C6B-C8B	-2.88	123.08	126.59
8	D	602	F43	CAB-C3B-C2B	-2.83	113.11	119.09
8	G	605	F43	O8D-C7D-C6D	-2.80	116.28	120.86
8	D	602	F43	O7B-C6B-C8B	-2.80	123.18	126.59
8	G	605	F43	C2B-C1B-NB	2.76	105.97	101.84
8	D	602	F43	C9A-C2A-C3A	2.68	116.94	112.98
8	J	602	F43	O7B-C6B-C8B	-2.67	123.33	126.59
8	A	606	F43	C9A-C2A-C3A	2.64	116.88	112.98
8	A	606	F43	O7B-C6B-C8B	-2.63	123.38	126.59
8	A	606	F43	CAB-C3B-C2B	-2.48	113.84	119.09
8	A	606	F43	C2B-C1B-NB	2.44	105.48	101.84
6	A	603	COM	O2S-S2-O1S	-2.42	105.56	113.95
8	G	605	F43	CAB-C3B-C2B	-2.39	114.03	119.09
6	J	601	COM	O2S-S2-C2	2.39	109.79	106.92
8	A	606	F43	C6D-C7D-CHD	2.37	121.42	116.95
6	D	601	COM	O3S-S2-O1S	-2.35	105.53	111.27
8	J	602	F43	C4D-ND-C1D	2.34	111.59	108.51
8	J	602	F43	C2A-C3A-C4A	-2.33	98.80	102.36
8	J	602	F43	C9D-C3D-C4D	-2.31	108.57	114.67
8	J	602	F43	C5C-C2C-C3C	-2.27	109.14	114.94
8	G	605	F43	C6D-C7D-CHD	2.26	121.21	116.95
8	G	605	F43	CAB-CBB-CCB	-2.25	108.75	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	602	F43	C5D-C6D-C7D	-2.14	107.92	113.55
6	D	601	COM	C2-C1-S1	-2.10	107.77	113.10
8	G	605	F43	CAA-CBA-CCA	-2.09	109.09	113.59
8	J	602	F43	CAB-C3B-C2B	-2.07	114.70	119.09
8	D	602	F43	C4D-ND-C1D	2.07	111.24	108.51
8	G	605	F43	CAD-C9D-C3D	-2.06	111.70	115.91
8	D	602	F43	C2B-C1B-NB	2.05	104.90	101.84
8	D	602	F43	CAB-CBB-CCB	-2.04	109.20	113.59
8	A	606	F43	CAB-CBB-CCB	-2.03	109.22	113.59
8	G	605	F43	C4D-ND-C1D	2.01	111.16	108.51
8	G	605	F43	C9B-C2B-C8B	-2.01	105.38	110.45

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
8	A	606	F43	C2D-C3D-C9D-CAD
4	A	601	GOL	O1-C1-C2-O2
8	J	602	F43	C3A-CAA-CBA-CCA
8	A	606	F43	C3A-CAA-CBA-CCA
8	D	602	F43	C3A-CAA-CBA-CCA
8	G	605	F43	C3A-CAA-CBA-CCA
7	G	604	TP7	C2-C3-C4-C5
7	A	604	TP7	CB-O4P-P-O3P
7	G	603	TP7	C2-C3-C4-C5

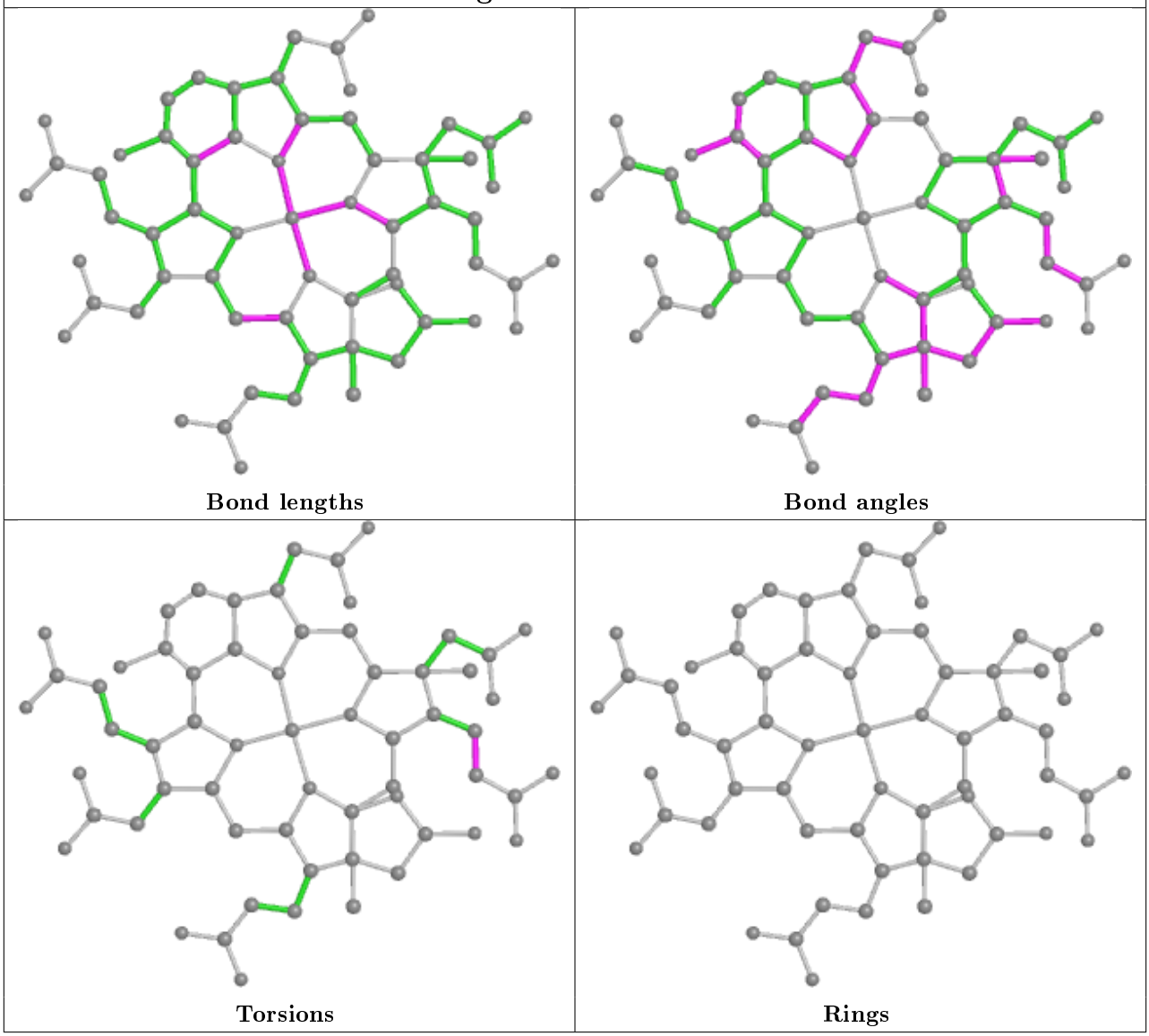
There are no ring outliers.

9 monomers are involved in 15 short contacts:

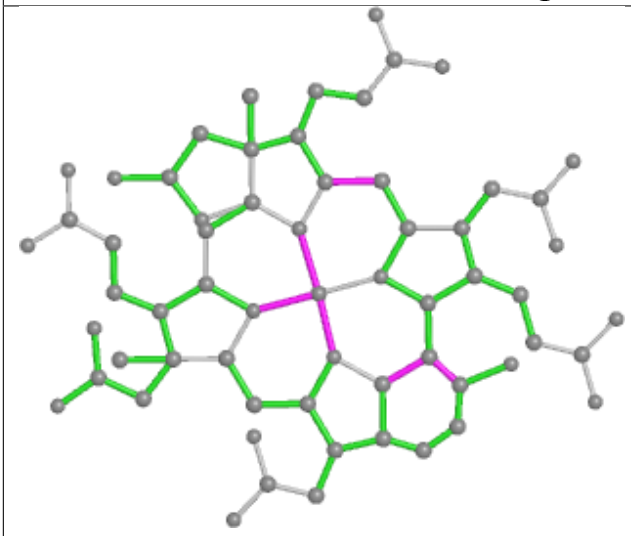
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	605	F43	4	0
8	J	602	F43	3	0
9	E	501	SO4	1	0
8	A	606	F43	2	0
6	G	602	COM	3	0
6	J	601	COM	3	0
8	D	602	F43	1	0
7	A	604	TP7	1	0
6	D	601	COM	2	0

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.

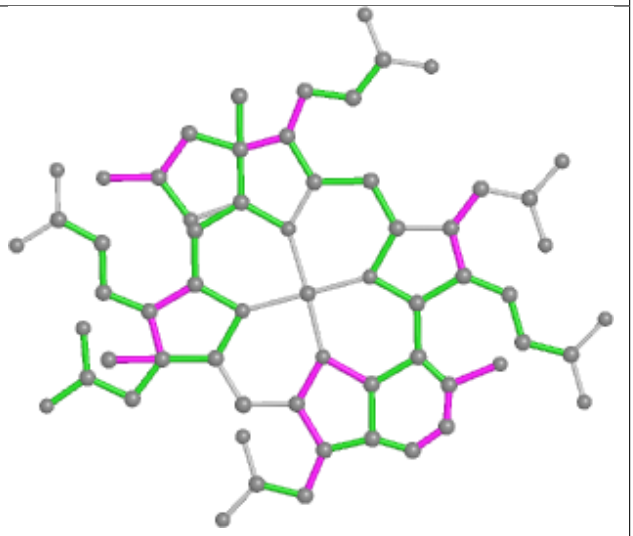
Ligand F43 G 605



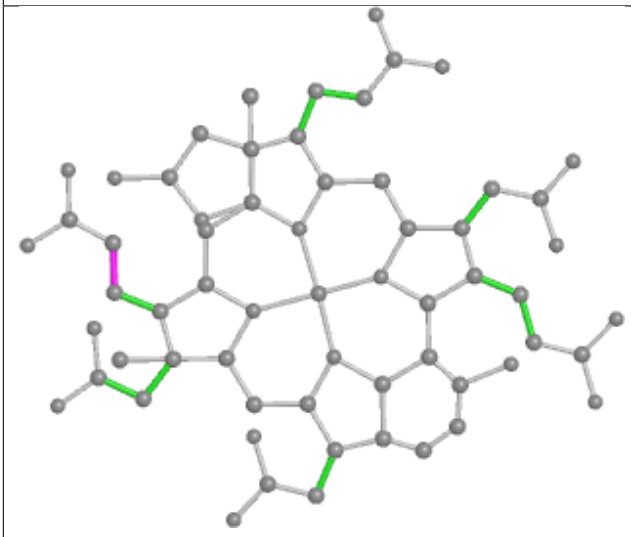
Ligand F43 J 602



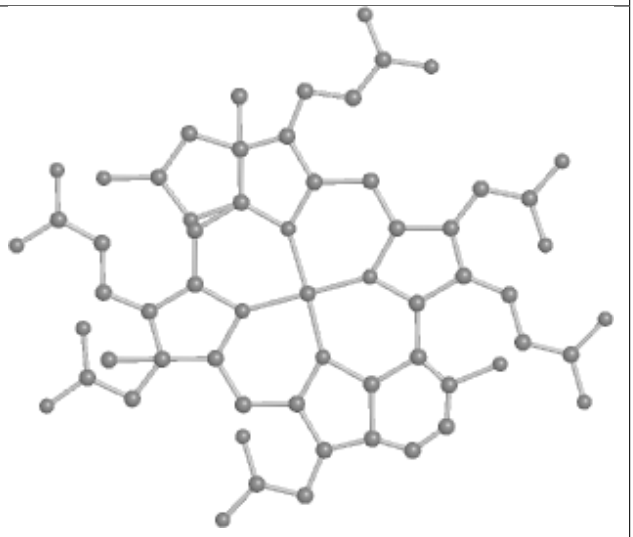
Bond lengths



Bond angles

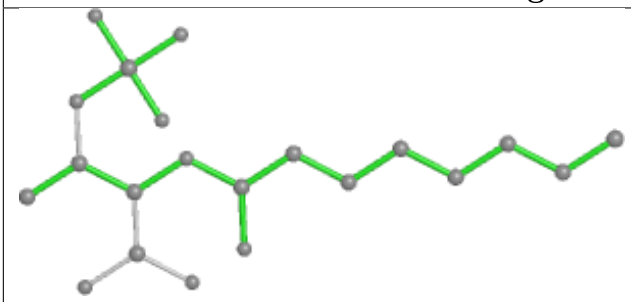


Torsions

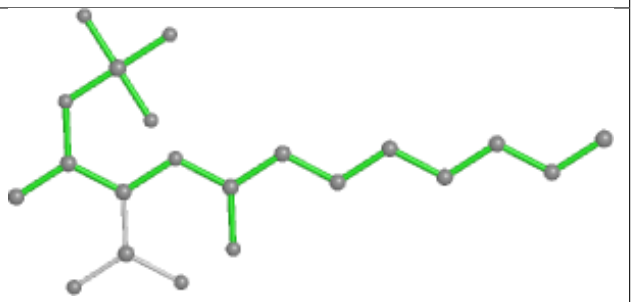


Rings

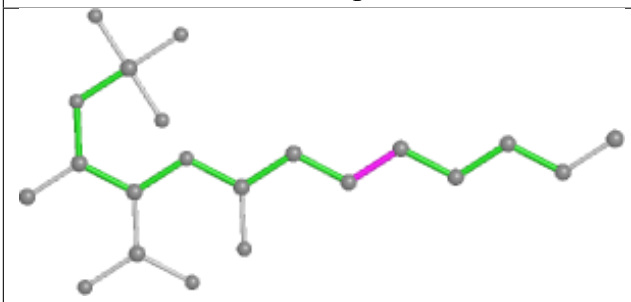
Ligand TP7 G 604



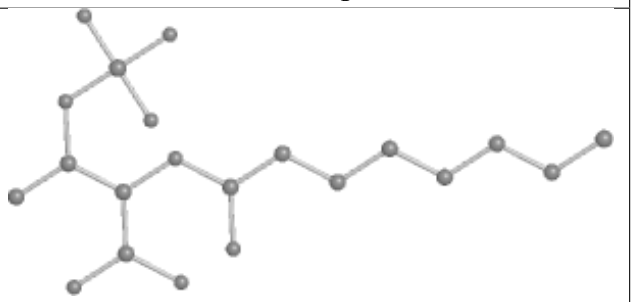
Bond lengths



Bond angles

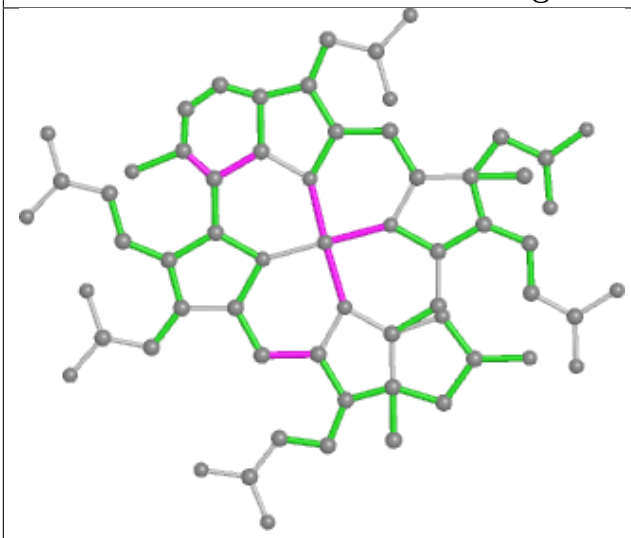


Torsions

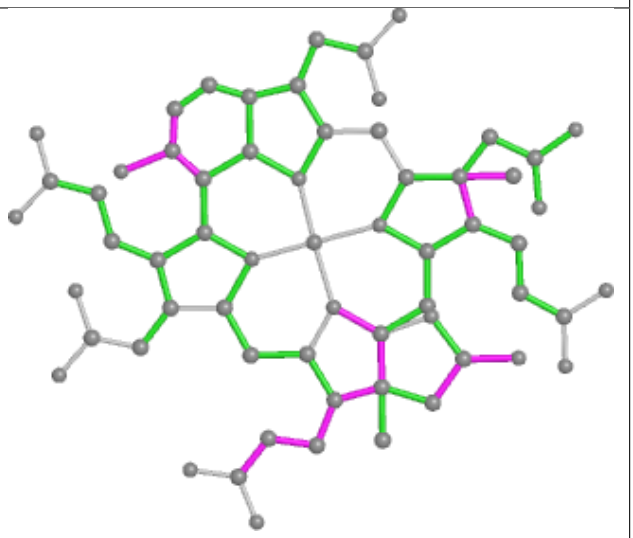


Rings

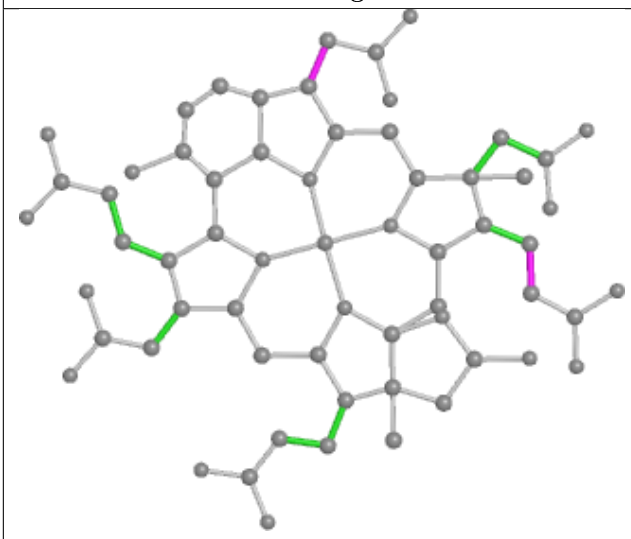
Ligand F43 A 606



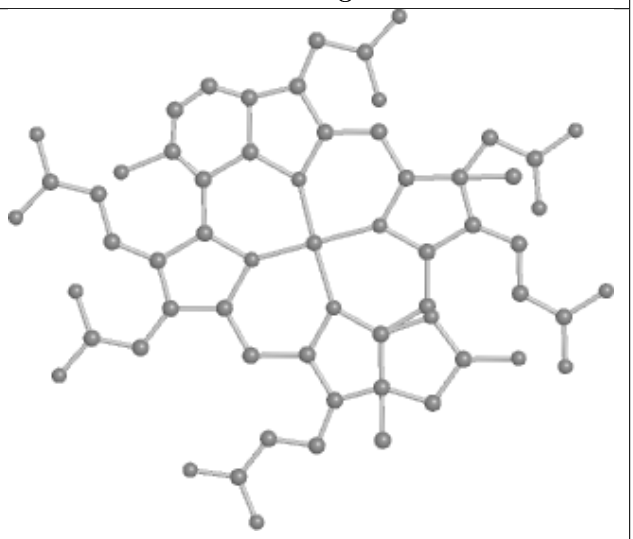
Bond lengths



Bond angles

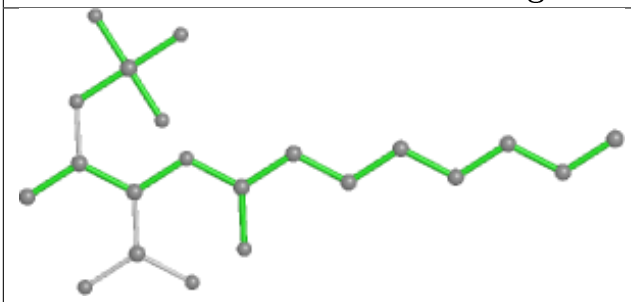


Torsions

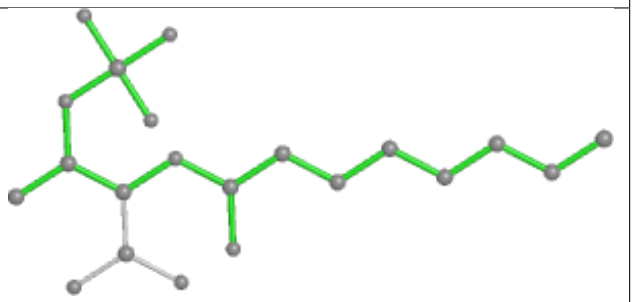


Rings

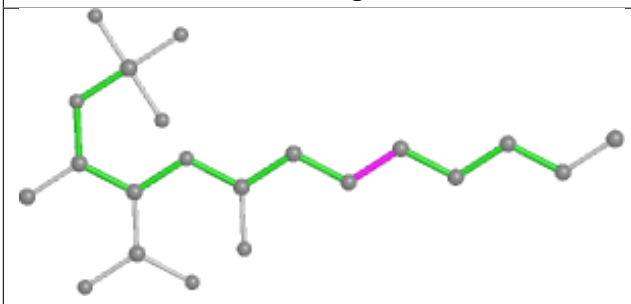
Ligand TP7 G 603



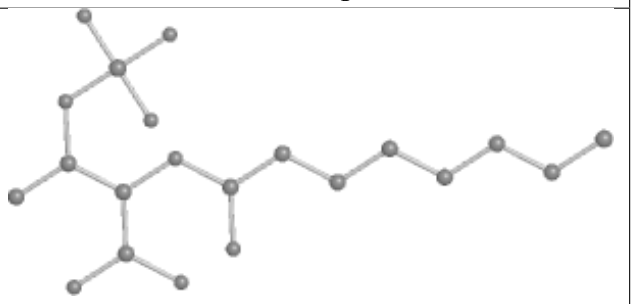
Bond lengths



Bond angles

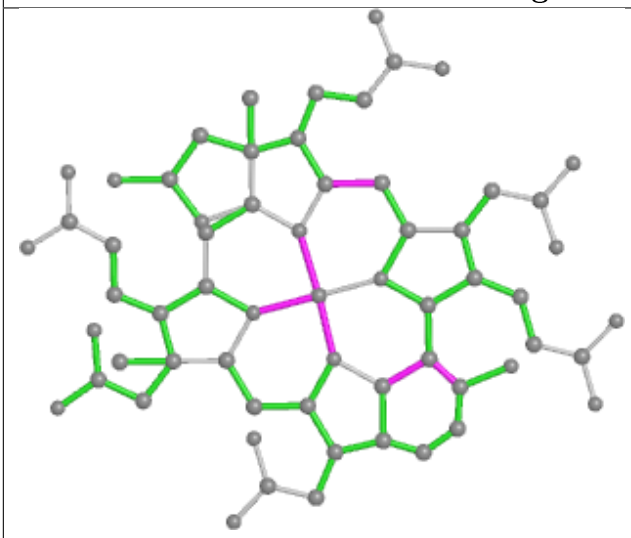


Torsions

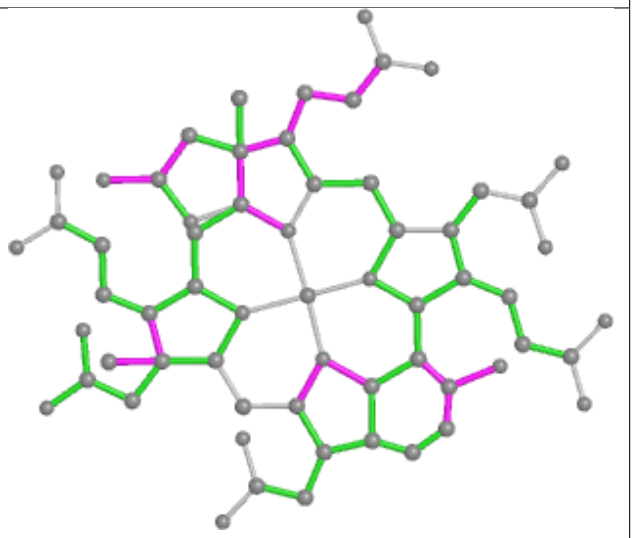


Rings

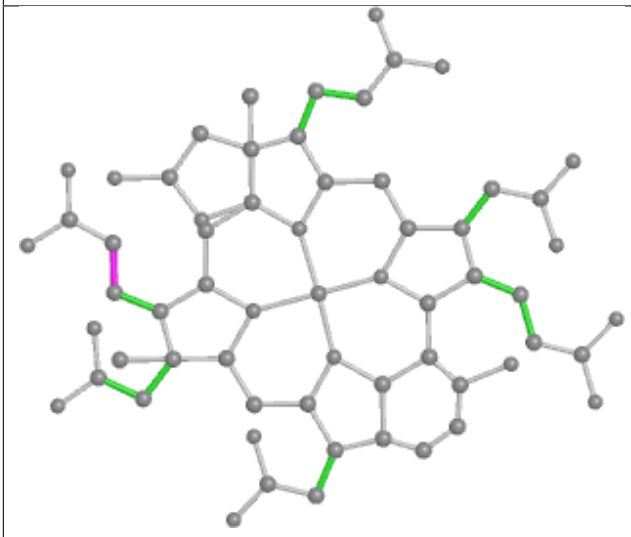
Ligand F43 D 602



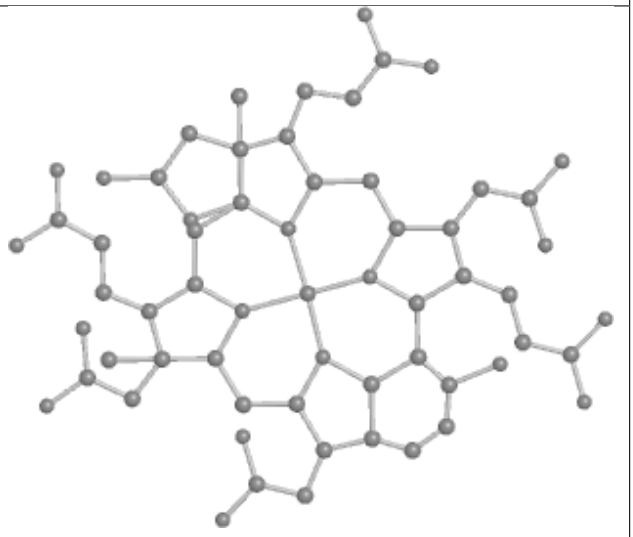
Bond lengths



Bond angles

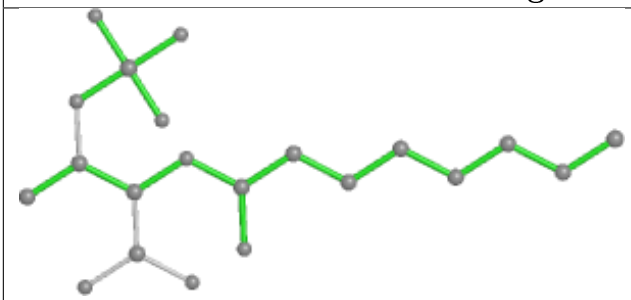


Torsions

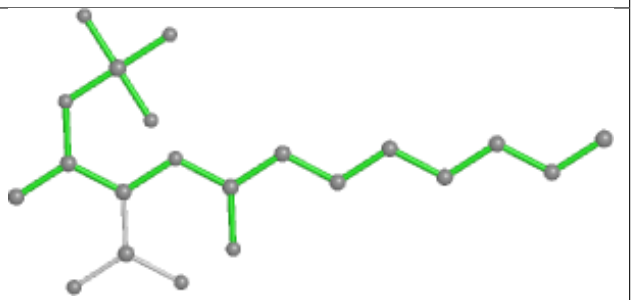


Rings

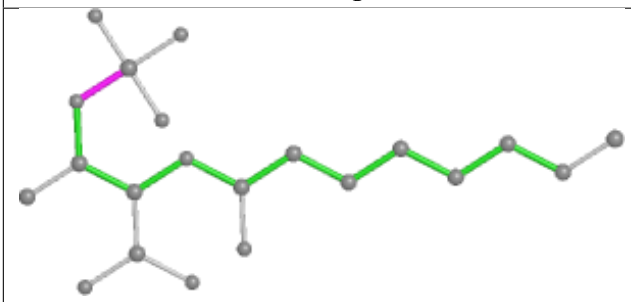
Ligand TP7 A 604



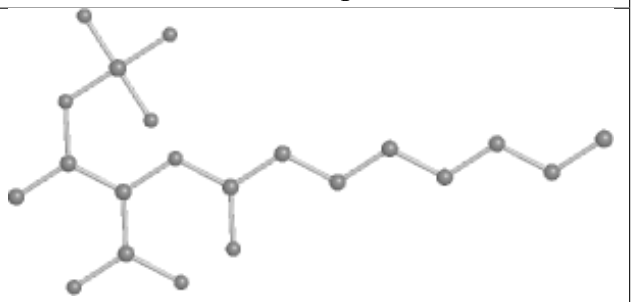
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	561/569 (98%)	-0.18	3 (0%) 91 90	14, 18, 28, 46	0
1	D	562/569 (98%)	-0.17	4 (0%) 87 87	14, 19, 31, 52	0
1	G	559/569 (98%)	0.79	77 (13%) 2 2	20, 46, 77, 89	0
1	J	560/569 (98%)	0.36	33 (5%) 22 20	17, 34, 76, 95	0
2	B	432/433 (99%)	-0.11	4 (0%) 84 84	15, 23, 33, 42	0
2	E	432/433 (99%)	-0.20	1 (0%) 95 94	16, 22, 32, 43	0
2	H	432/433 (99%)	0.65	46 (10%) 6 5	22, 38, 66, 87	0
2	K	432/433 (99%)	0.77	47 (10%) 5 4	28, 48, 74, 104	0
3	C	247/248 (99%)	-0.16	6 (2%) 59 56	16, 22, 37, 52	0
3	F	247/248 (99%)	-0.15	2 (0%) 86 86	17, 23, 35, 42	0
3	I	238/248 (95%)	0.84	23 (9%) 7 6	27, 54, 74, 88	0
3	L	246/248 (99%)	1.26	43 (17%) 1 1	38, 72, 102, 120	0
All	All	4948/5000 (98%)	0.27	289 (5%) 23 20	14, 28, 73, 120	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	2	ALA	7.8
2	K	2	SER	7.4
2	K	55	ALA	6.7
3	F	2	ALA	6.3
1	G	194	ILE	5.7
3	C	2	ALA	5.5
2	K	280	VAL	5.5
2	H	284	ALA	5.3
2	K	433	LEU	5.2
3	I	64	ASP	5.2
3	I	49	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	G	214	ILE	4.9
1	G	405	TYR	4.9
1	G	190	LEU	4.8
1	G	196	LYS	4.8
2	K	364	TYR	4.8
1	G	142	VAL	4.7
1	G	212	ALA	4.6
2	K	76	ALA	4.5
1	G	218	ILE	4.5
2	K	359	PHE	4.5
1	J	63	ALA	4.4
2	H	2	SER	4.4
3	L	194	LEU	4.4
1	G	191	ALA	4.4
3	L	100	TYR	4.4
2	K	70	MET	4.3
1	G	193	GLU	4.3
1	J	568	ALA	4.2
1	A	5	ASP	4.2
3	L	118	LEU	4.2
2	K	358	PHE	4.2
3	I	45	ALA	4.1
2	K	142	PHE	4.0
3	I	48	SER	4.0
3	L	55	PRO	4.0
1	G	532	ALA	4.0
1	J	64	ALA	4.0
2	H	74	ILE	4.0
3	L	49	ASP	3.9
2	H	283	VAL	3.9
1	G	199	LEU	3.9
3	I	66	PRO	3.9
1	G	189	GLU	3.8
1	G	202	ILE	3.8
1	G	32	THR	3.8
1	G	31	SER	3.8
2	K	141	LEU	3.8
3	L	58	ALA	3.8
1	D	5	ASP	3.8
2	K	363	ILE	3.7
2	K	354	VAL	3.7
1	G	185	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	K	14	LEU	3.7
1	G	516	GLY	3.6
1	G	388	VAL	3.6
2	H	80	ARG	3.6
1	G	144	PRO	3.6
2	K	72	LEU	3.6
2	K	143	ASP	3.5
1	G	204	LYS	3.5
1	G	145	GLU	3.5
2	H	147	PHE	3.5
1	G	220	LYS	3.5
3	I	211	LYS	3.5
2	K	80	ARG	3.5
2	K	282	LYS	3.5
2	H	290	PHE	3.5
2	K	73	ASP	3.5
1	G	529	VAL	3.4
1	J	34	ILE	3.4
1	G	222	THR	3.4
2	H	398	ALA	3.4
3	L	197	LYS	3.4
3	I	47	GLY	3.4
1	G	147	ILE	3.4
2	K	273	LEU	3.3
3	I	50	TYR	3.3
3	C	64	ASP	3.3
2	H	76	ALA	3.3
1	G	138	LEU	3.3
2	H	13	LYS	3.3
3	F	49	ASP	3.3
2	K	71	LYS	3.2
3	L	211	LYS	3.2
1	J	376	GLY	3.2
1	J	67	GLY	3.2
2	K	288	TYR	3.2
3	L	7	TYR	3.2
3	C	61	GLY	3.2
2	E	433	LEU	3.2
1	J	461	PHE	3.2
1	J	139	GLY	3.2
2	H	12	GLY	3.2
3	I	46	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	466	LEU	3.1
2	H	248	VAL	3.1
1	J	23	GLY	3.1
3	L	180	GLY	3.1
3	C	60	MET	3.1
3	L	64	ASP	3.1
2	K	147	PHE	3.1
3	L	8	TYR	3.1
2	H	419	ILE	3.0
2	H	73	ASP	3.0
1	G	186	GLY	3.0
1	J	370	TYR	3.0
3	L	123	ILE	3.0
2	H	30	ARG	3.0
1	J	459	LEU	3.0
3	L	88	TRP	3.0
1	J	337	LEU	3.0
3	L	14	VAL	3.0
2	H	282	LYS	2.9
2	H	354	VAL	2.9
3	L	229	VAL	2.9
1	G	371	ALA	2.9
1	D	569	LYS	2.9
1	G	192	ASP	2.9
1	G	200	ILE	2.9
2	H	146	ILE	2.9
2	H	288	TYR	2.9
3	L	198	VAL	2.8
1	G	203	ASP	2.8
1	G	568	ALA	2.8
1	G	188	ASP	2.8
1	G	223	TRP	2.8
3	L	193	PRO	2.8
3	I	195	ASP	2.8
3	I	222	PRO	2.8
2	H	11	ARG	2.7
1	J	36	SER	2.7
2	B	378	VAL	2.7
1	G	139	GLY	2.7
2	K	52	LYS	2.7
1	J	466	LEU	2.7
3	L	131	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	377	ILE	2.7
1	G	208	GLU	2.7
2	H	280	VAL	2.7
3	L	151	LEU	2.7
1	G	184	PHE	2.7
2	H	239	TYR	2.6
2	K	291	TYR	2.6
1	G	211	ALA	2.6
1	G	312	ARG	2.6
2	K	377	ILE	2.6
1	G	373	ASP	2.6
3	I	11	ASN	2.6
1	J	366	TYR	2.6
2	K	302	TYR	2.6
1	G	217	ALA	2.6
2	H	410	ALA	2.6
1	G	12	LYS	2.6
3	I	63	PRO	2.6
2	K	74	ILE	2.6
2	H	101	VAL	2.6
1	J	24	GLU	2.5
3	L	165	GLU	2.5
1	G	525	PRO	2.5
1	D	568	ALA	2.5
1	G	216	ALA	2.5
2	K	18	ASP	2.5
1	G	143	THR	2.5
3	L	124	VAL	2.5
3	L	163	LEU	2.5
2	H	417	GLY	2.5
3	I	75	PRO	2.5
3	I	207	GLU	2.5
1	J	32	THR	2.5
1	J	96	ASP	2.5
1	G	215	LYS	2.5
2	K	75	VAL	2.5
1	G	534	PRO	2.4
2	H	77	ASN	2.4
1	G	372	VAL	2.4
2	H	313	VAL	2.4
3	I	71	VAL	2.4
3	C	57	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	19	THR	2.4
2	K	287	GLY	2.4
1	J	47	ALA	2.4
3	L	200	LEU	2.4
1	G	207	GLY	2.4
2	B	2	SER	2.4
2	H	250	GLU	2.4
1	G	285	LEU	2.4
1	J	452	LEU	2.4
2	H	14	LEU	2.4
2	H	72	LEU	2.4
3	L	56	PRO	2.4
1	G	195	ASP	2.4
1	G	13	ALA	2.4
3	L	45	ALA	2.4
2	K	48	GLY	2.4
1	G	368	TYR	2.3
1	J	464	TYR	2.3
3	L	50	TYR	2.3
2	H	83	GLU	2.3
1	J	22	TRP	2.3
2	K	284	ALA	2.3
1	G	459	LEU	2.3
3	L	209	ALA	2.3
1	G	35	THR	2.3
2	H	75	VAL	2.3
2	H	269	VAL	2.3
3	I	218	VAL	2.3
3	L	168	VAL	2.3
1	J	208	GLU	2.3
1	G	201	ASP	2.3
2	K	356	PHE	2.3
1	D	32	THR	2.3
1	J	81	PRO	2.3
3	L	202	LYS	2.3
2	K	93	GLU	2.3
2	H	18	ASP	2.3
1	J	91	VAL	2.3
2	B	354	VAL	2.3
3	L	117	THR	2.3
2	H	253	LYS	2.3
2	K	378	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	2.2
1	J	28	THR	2.2
2	K	261	ILE	2.2
1	G	219	GLY	2.2
2	K	355	GLY	2.2
3	L	208	GLU	2.2
1	J	373	ASP	2.2
3	C	195	ASP	2.2
2	K	328	LEU	2.2
1	G	542	GLN	2.2
3	L	212	ARG	2.2
3	I	232	TRP	2.2
2	H	279	SER	2.2
1	G	406	PHE	2.2
3	I	97	ALA	2.2
1	G	153	VAL	2.2
1	G	9	LEU	2.2
1	A	189	GLU	2.2
1	G	315	ASP	2.2
3	I	4	GLU	2.2
2	H	278	ILE	2.2
2	K	164	ILE	2.2
3	I	248	GLN	2.2
1	J	18	PHE	2.2
1	J	375	TYR	2.2
1	G	187	ASP	2.2
2	K	277	VAL	2.2
1	G	376	GLY	2.2
1	J	207	GLY	2.2
1	G	206	PHE	2.1
1	J	57	GLN	2.1
3	L	104	TYR	2.1
3	L	179	GLU	2.1
3	L	51	PRO	2.1
1	J	19	THR	2.1
2	H	33	ARG	2.1
3	I	209	ALA	2.1
3	L	60	MET	2.1
2	H	79	GLU	2.1
2	K	201	GLN	2.1
2	H	329	LEU	2.1
1	G	209	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	359	PHE	2.1
1	G	30	VAL	2.1
1	G	313	VAL	2.1
2	H	93	GLU	2.1
1	G	239	ALA	2.1
3	L	107	ALA	2.1
3	L	173	LEU	2.1
1	G	7	GLU	2.1
1	G	311	ASP	2.1
1	J	30	VAL	2.1
2	H	52	LYS	2.1
2	H	430	ALA	2.1
3	L	156	VAL	2.1
3	L	215	ILE	2.1
1	G	148	ASN	2.0
1	G	423	VAL	2.0
2	K	19	VAL	2.0
2	H	433	LEU	2.0
2	K	329	LEU	2.0
2	K	16	ALA	2.0
2	K	53	ALA	2.0
2	K	103	ALA	2.0
3	L	59	GLU	2.0
2	H	411	VAL	2.0
1	G	461	PHE	2.0
3	L	199	ASP	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, 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
1	MHS	D	275	11/12	0.89	0.13	17,20,23,23	0
1	AGM	J	289	12/13	0.90	0.16	23,24,25,25	0
1	MHS	G	275	11/12	0.91	0.10	35,35,38,38	0
1	AGM	G	289	12/13	0.92	0.16	21,21,23,23	0
1	MHS	A	275	11/12	0.92	0.10	15,18,20,20	0
1	AGM	D	289	12/13	0.93	0.15	15,15,16,16	0
1	AGM	A	289	12/13	0.94	0.14	15,15,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHS	J	275	11/12	0.95	0.11	19,22,22,22	0
1	GL3	J	463	4/5	0.96	0.18	36,37,38,38	0
1	GL3	G	463	4/5	0.98	0.11	29,30,30,30	0
1	GL3	A	463	4/5	0.99	0.14	14,15,15,15	0
1	GL3	D	463	4/5	0.99	0.11	15,16,16,16	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

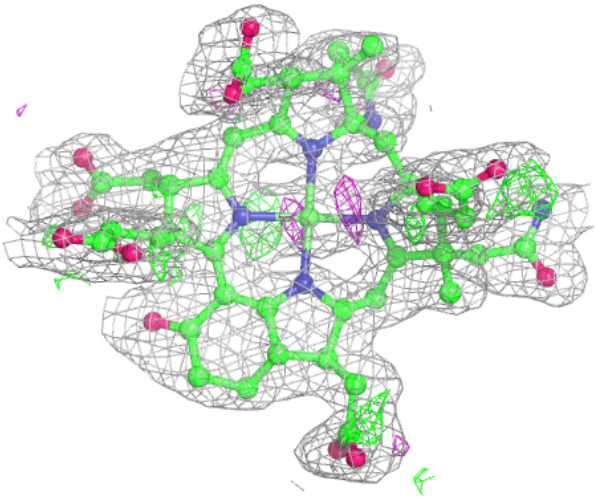
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

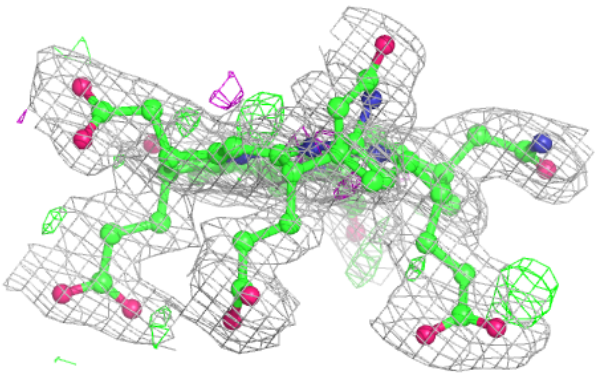
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	601	6/6	0.83	0.14	73,73,73,73	0
9	SO4	K	501	5/5	0.83	0.17	96,96,96,96	0
9	SO4	H	501	5/5	0.85	0.32	43,43,44,44	5
4	GOL	E	502	6/6	0.85	0.14	32,35,35,35	0
4	GOL	B	502	6/6	0.87	0.18	33,35,35,36	0
9	SO4	B	501	5/5	0.87	0.22	33,33,34,34	5
9	SO4	E	501	5/5	0.89	0.25	59,59,59,59	0
9	SO4	E	503	5/5	0.92	0.21	21,22,22,22	5
8	F43	G	605	62/62	0.94	0.12	36,40,43,44	0
7	TP7	G	604	21/21	0.96	0.17	30,31,34,35	0
6	COM	J	601	7/7	0.96	0.12	43,44,44,45	0
8	F43	J	602	62/62	0.96	0.10	22,25,28,30	0
7	TP7	G	603	21/21	0.96	0.15	23,24,26,27	0
6	COM	G	602	7/7	0.97	0.07	32,33,34,34	0
6	COM	A	603	7/7	0.97	0.09	20,21,21,22	0
8	F43	A	606	62/62	0.97	0.10	14,16,19,21	0
7	TP7	A	604	21/21	0.97	0.11	16,17,18,19	0
7	TP7	A	605	21/21	0.97	0.10	15,17,18,18	0
8	F43	D	602	62/62	0.98	0.11	14,16,17,18	0
6	COM	D	601	7/7	0.98	0.08	20,21,22,22	0
5	K	G	601	1/1	0.99	0.06	24,24,24,24	0
5	K	A	602	1/1	1.00	0.09	16,16,16,16	0

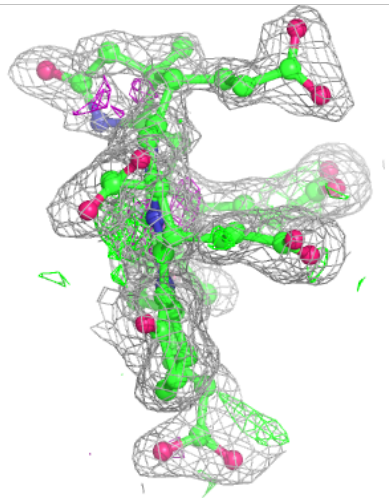
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around F43 G 605:

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

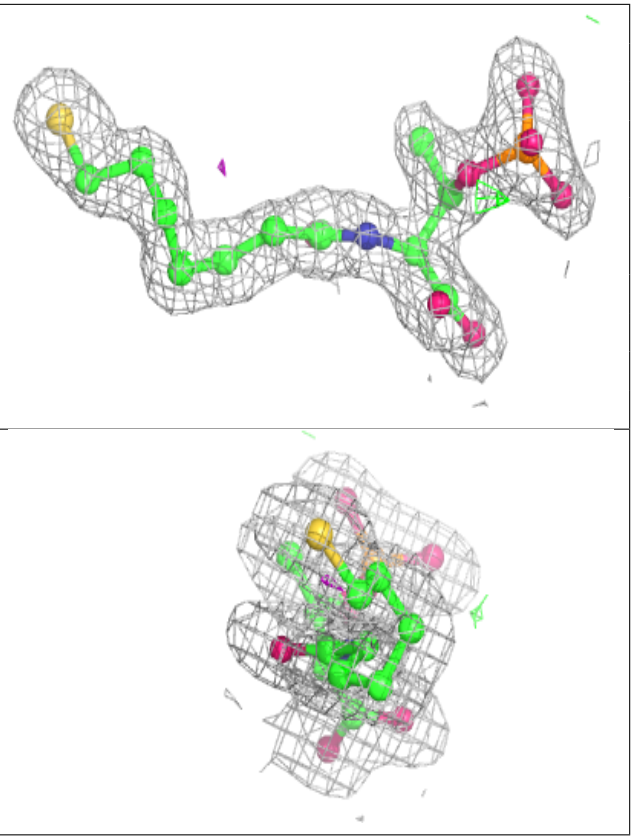


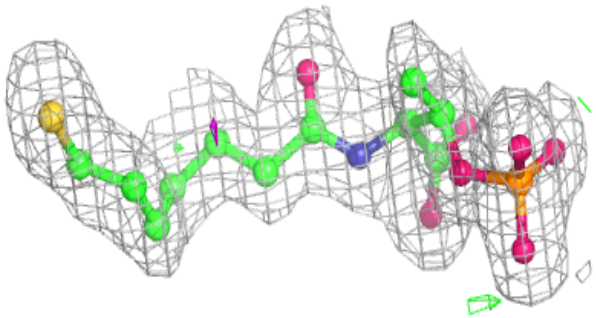




Electron density around TP7 G 604:

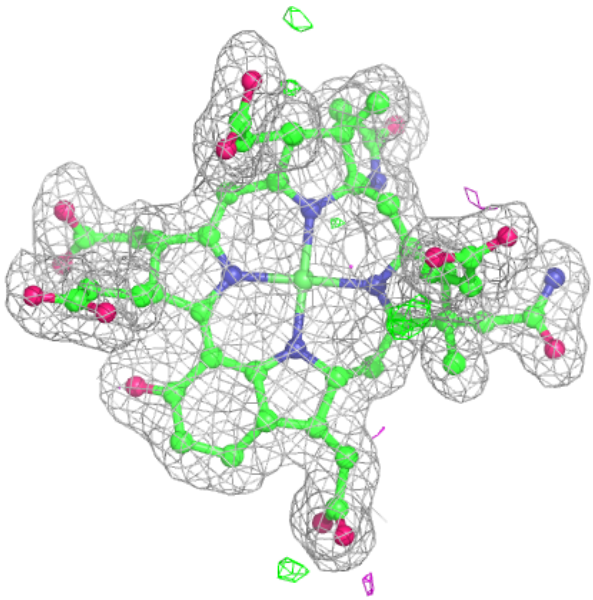
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

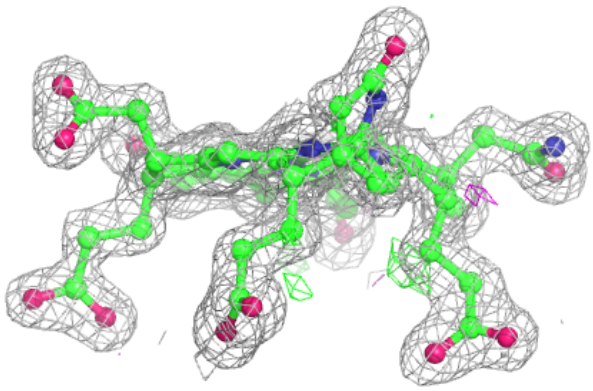


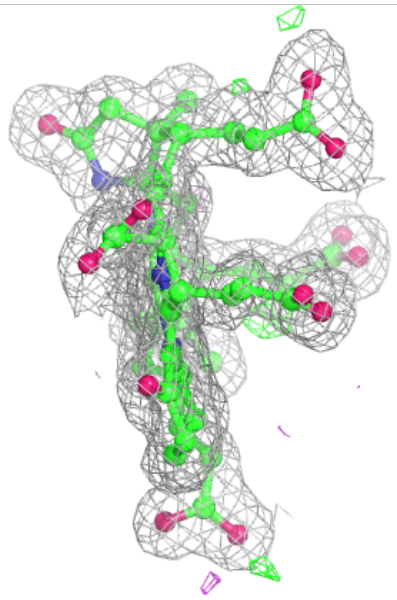


Electron density around F43 J 602:

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

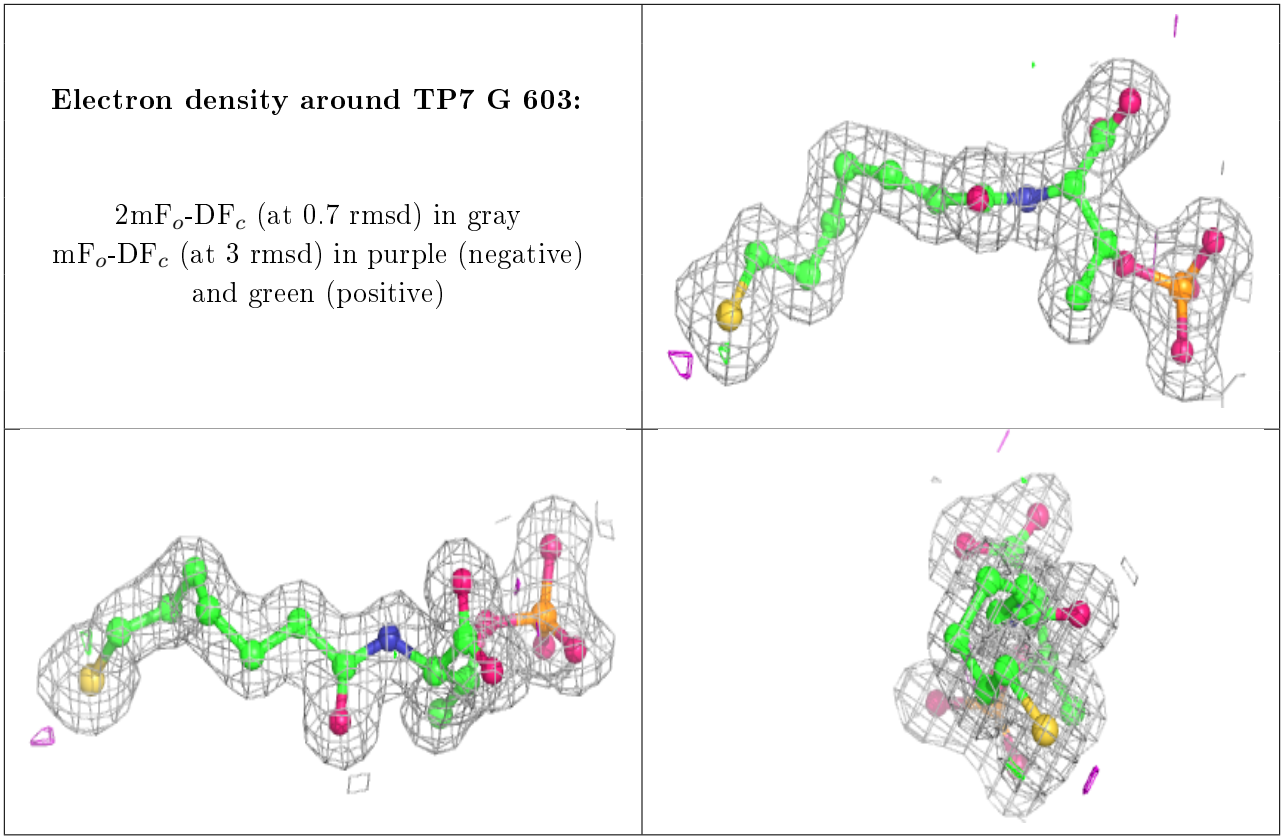






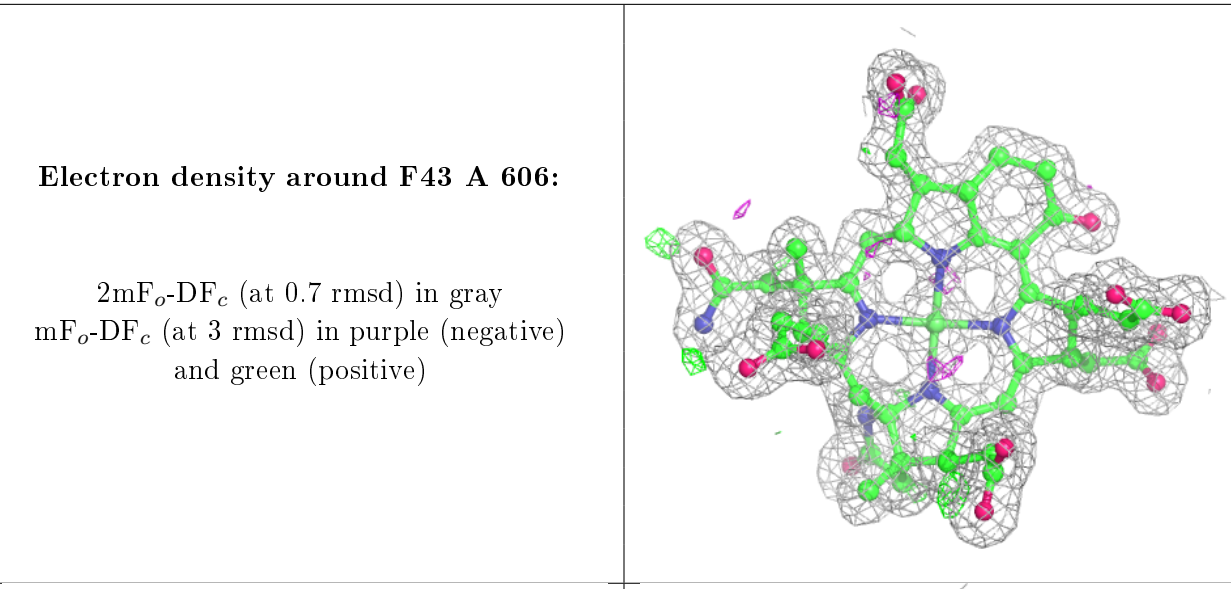
Electron density around TP7 G 603:

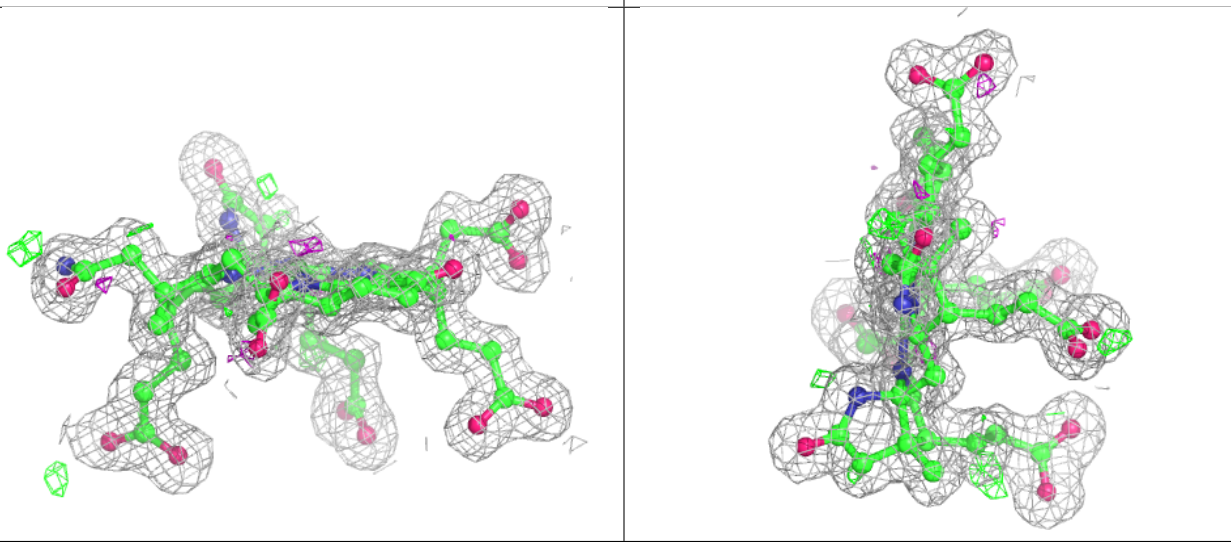
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around F43 A 606:

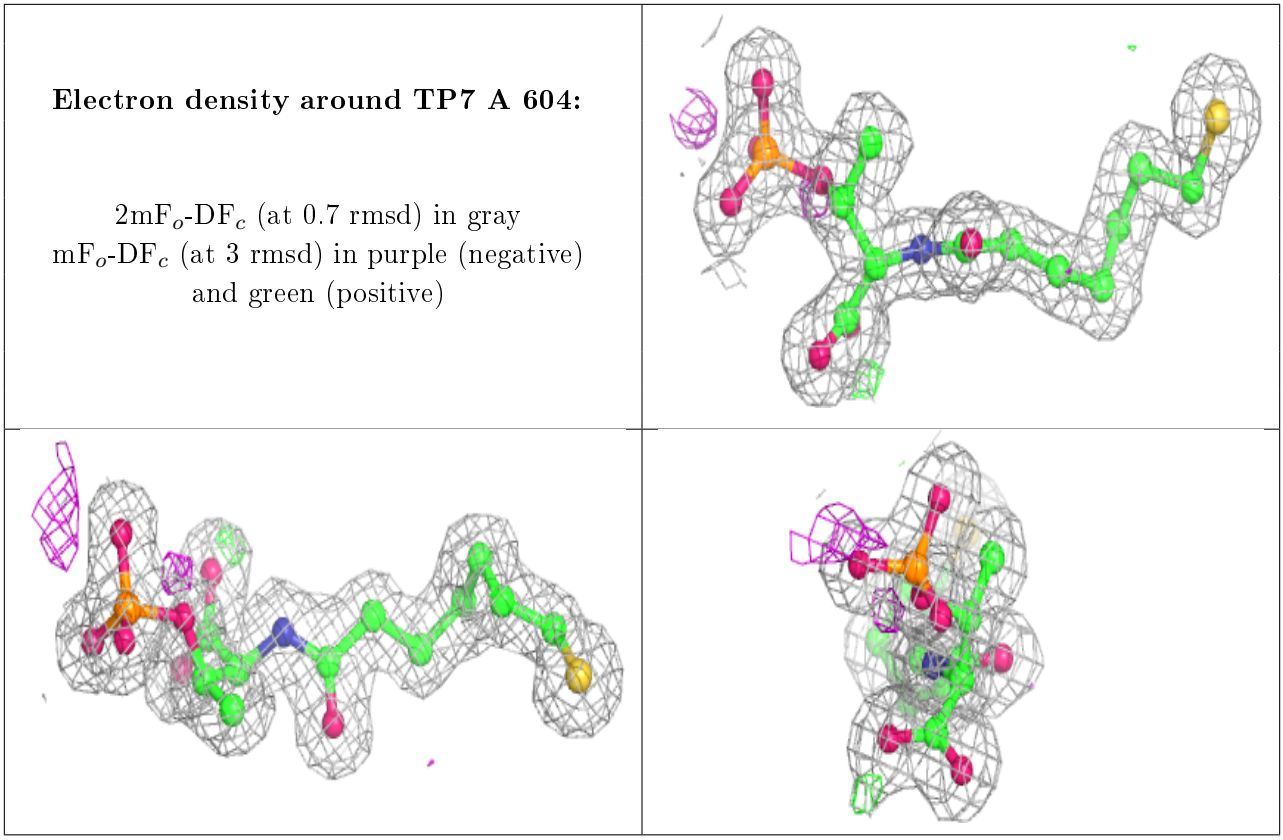
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





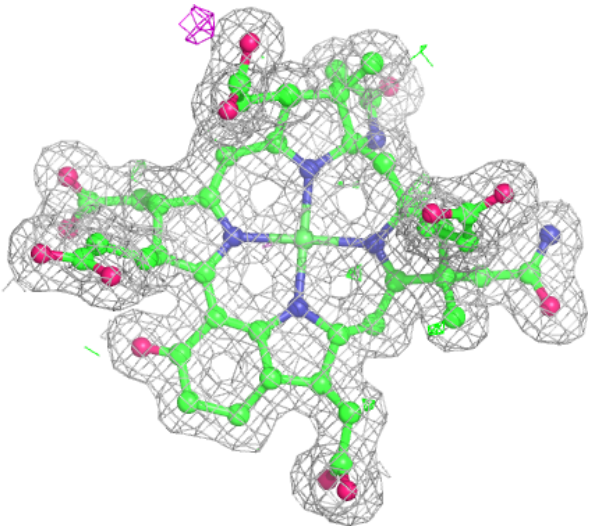
Electron density around TP7 A 604:

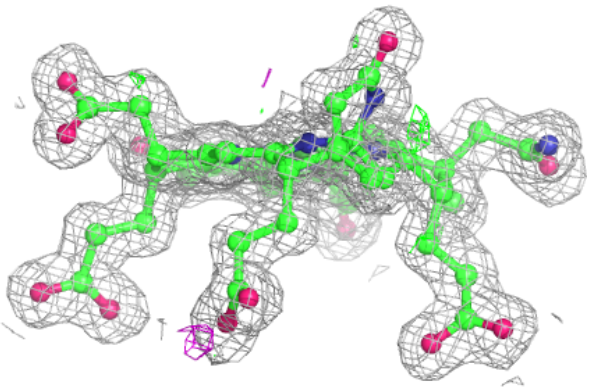
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

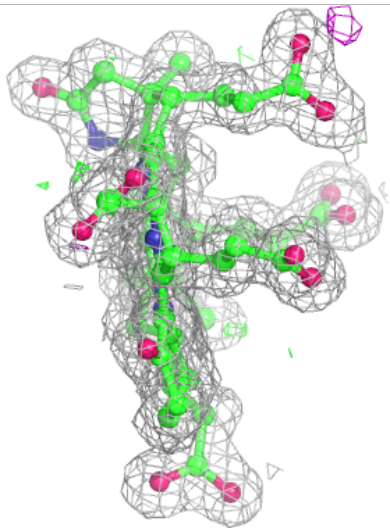


Electron density around F43 D 602:

$2mF_o$-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

There are no such residues in this entry.