wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 11:13 pm GMT

PDB ID	:	5A8W
Title	:	METHYL-COENZYME M REDUCTASE II FROM METHANOTHERMOBACTER WOLFEII AT 1. 8 A RESOLUTION
Authors	:	Wagner, T.; Ermler, U.
Deposited on	:	2015-07-17
Resolution	:	1.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

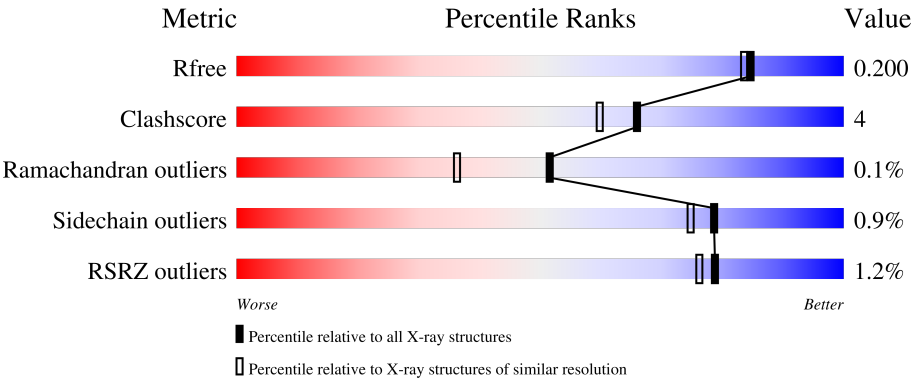
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	554	89% 9%
1	D	554	89% 10%
1	G	554	90% 8%
1	J	554	89% 10%
2	B	443	94% 5%

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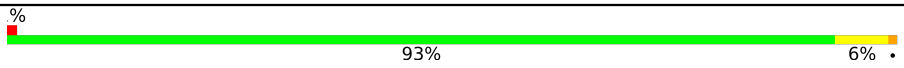
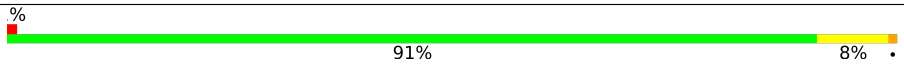
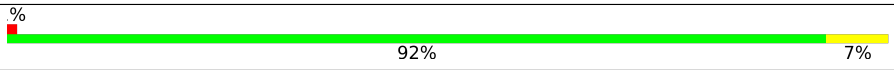
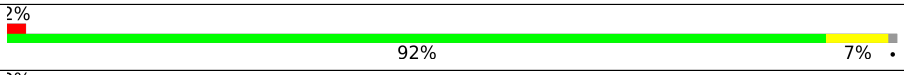
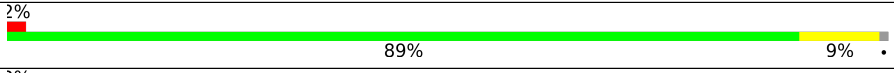
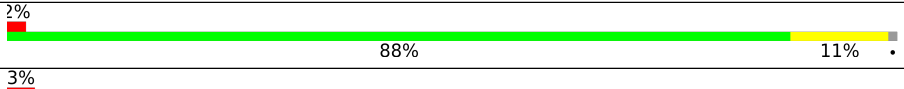
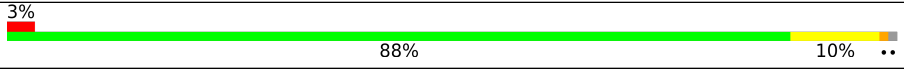
Mol	Chain	Length	Quality of chain
2	E	443	
2	H	443	
2	K	443	
3	C	265	
3	F	265	
3	I	265	
3	L	265	

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
4	COM	J	1555	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 42336 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 II REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	8	0
			4273	2703	720	827	23			
1	D	549	Total	C	N	O	S	0	7	0
			4276	2705	718	830	23			
1	G	548	Total	C	N	O	S	0	8	0
			4271	2701	717	830	23			
1	J	548	Total	C	N	O	S	0	8	0
			4273	2704	716	831	22			

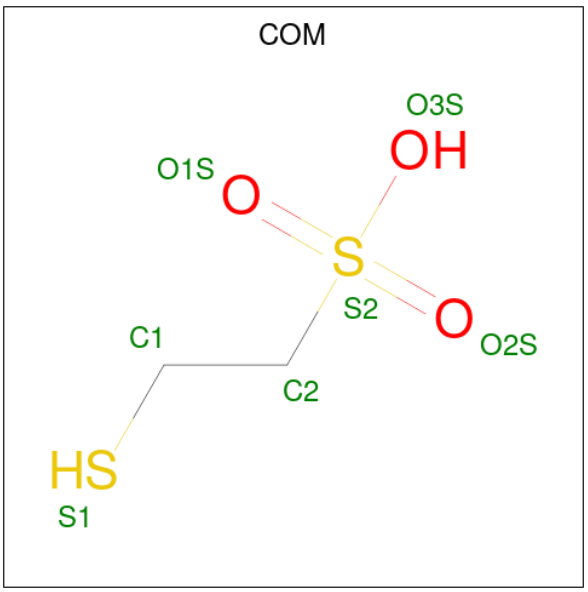
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	3	0
			3315	2101	558	642	14			
2	E	442	Total	C	N	O	S	0	4	0
			3319	2103	558	644	14			
2	H	442	Total	C	N	O	S	0	5	0
			3325	2108	560	643	14			
2	K	442	Total	C	N	O	S	0	8	0
			3348	2126	563	645	14			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE II.

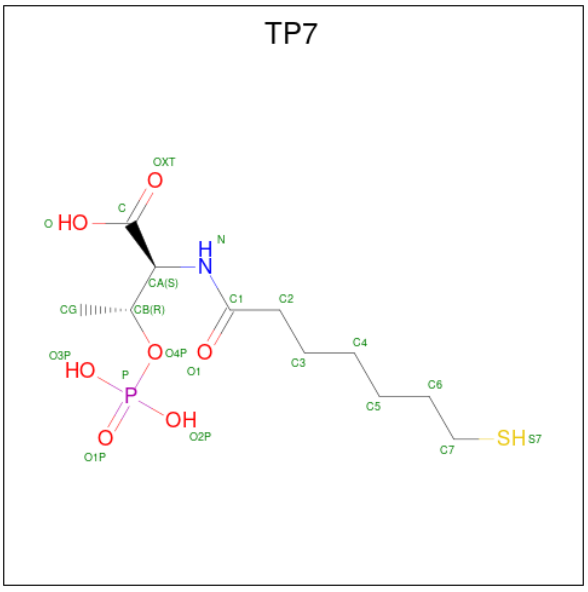
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	4	0
			2155	1340	382	423	10			
3	F	263	Total	C	N	O	S	0	2	0
			2147	1334	383	420	10			
3	I	263	Total	C	N	O	S	0	2	0
			2147	1335	383	419	10			
3	L	263	Total	C	N	O	S	0	5	0
			2167	1348	388	421	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



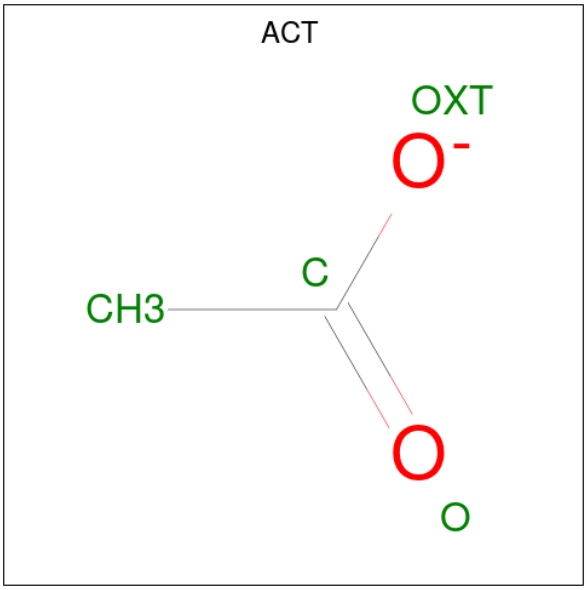
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		
4	D	1	Total	C	O	S	0	0
			7	2	3	2		
4	G	1	Total	C	O	S	0	0
			7	2	3	2		
4	J	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		

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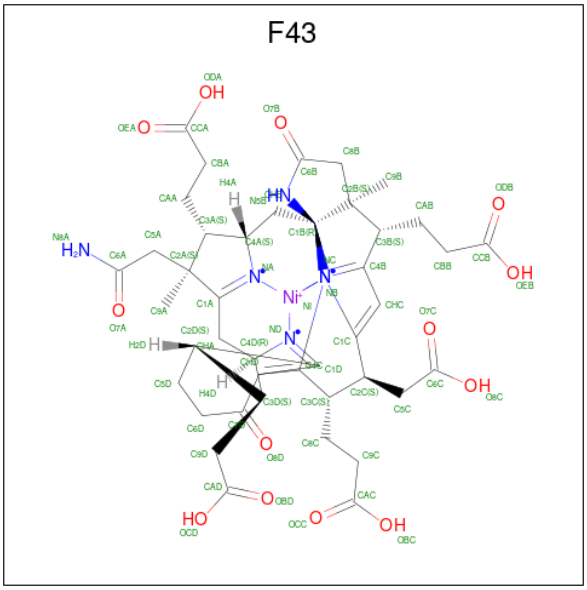
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0

- Molecule 7 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Na 1 1	0	0

- Molecule 9 is water.

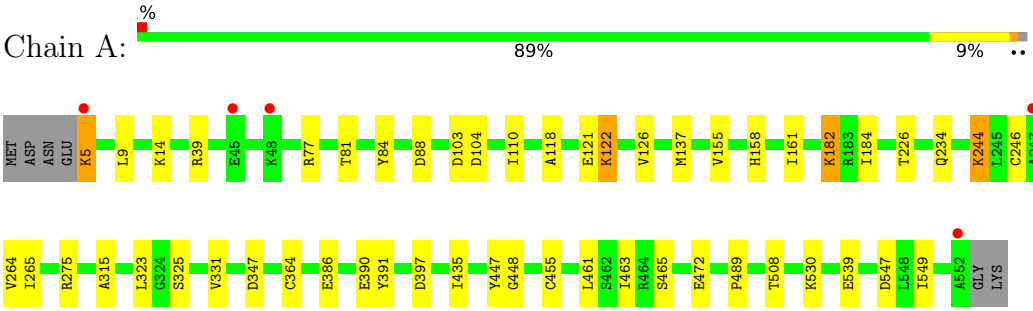
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	381	Total O 381 381	0	0
9	B	281	Total O 281 281	0	0
9	C	152	Total O 152 152	0	0
9	D	284	Total O 284 284	0	0
9	E	223	Total O 223 223	0	0
9	F	145	Total O 145 145	0	0
9	G	385	Total O 385 385	0	0
9	H	269	Total O 269 269	0	0
9	I	147	Total O 147 147	0	0
9	J	291	Total O 291 291	0	0
9	K	224	Total O 224 224	0	0
9	L	133	Total O 133 133	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.

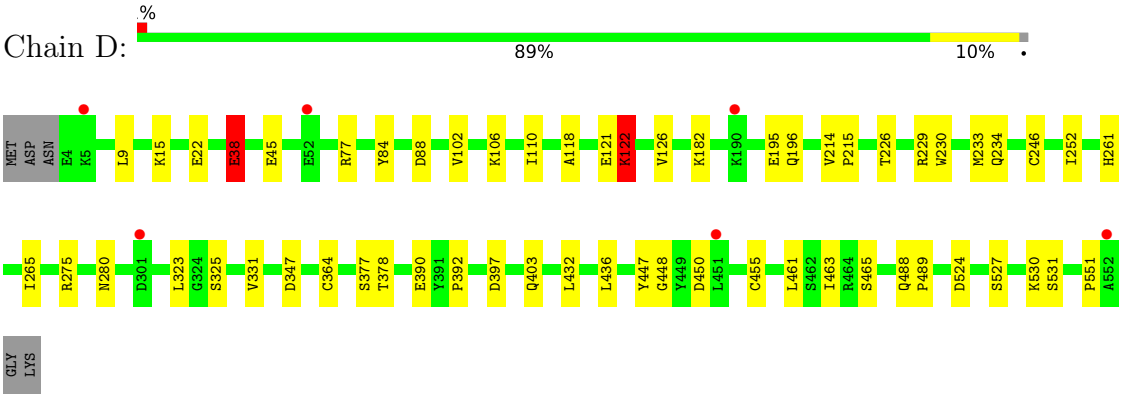
• Molecule 1: METHYL-COENZYME M II REDUCTASE

Chain A:



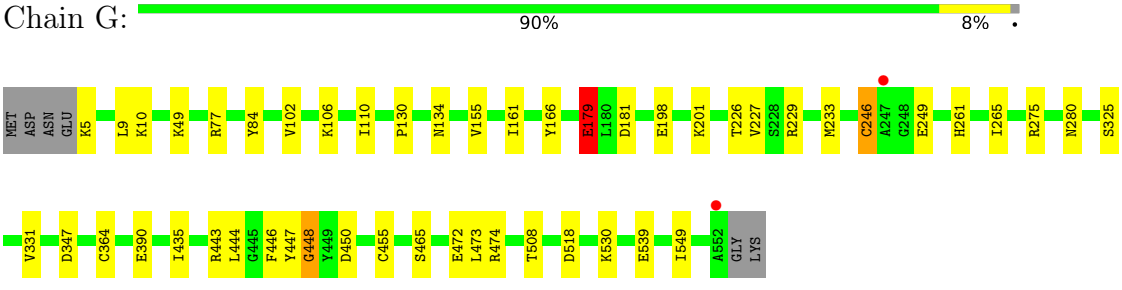
• Molecule 1: METHYL-COENZYME M II REDUCTASE

Chain D:



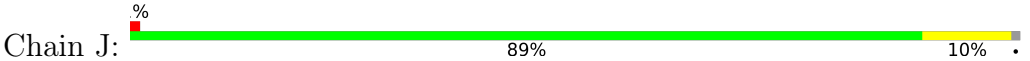
• Molecule 1: METHYL-COENZYME M II REDUCTASE

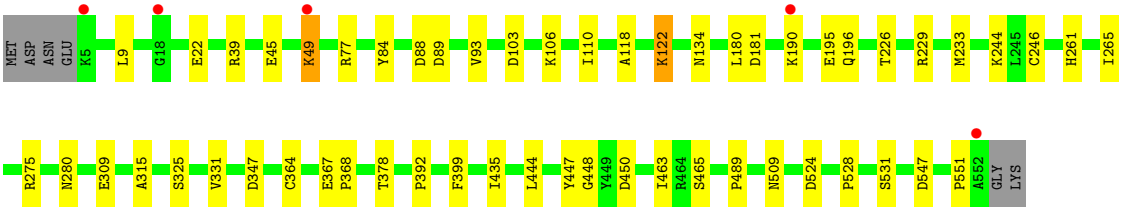
Chain G:



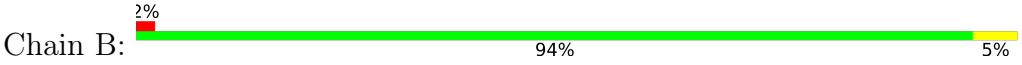
• Molecule 1: METHYL-COENZYME M II REDUCTASE

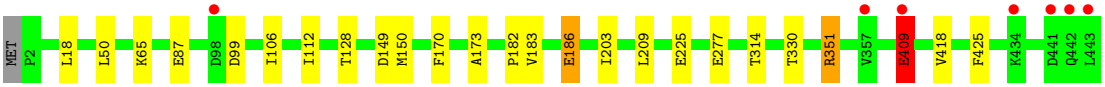
Chain J:



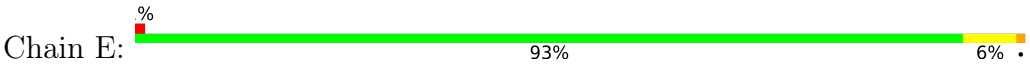


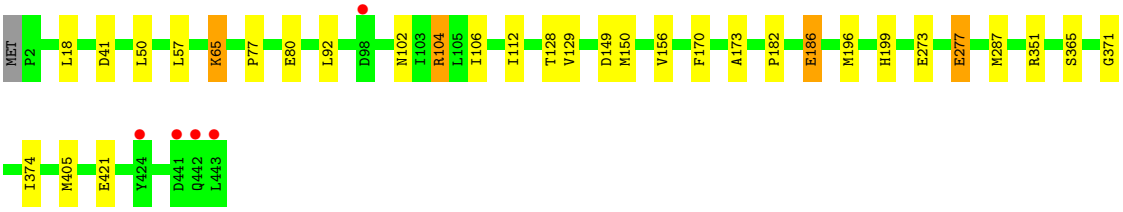
• Molecule 2: METHYL-COENZYME M REDUCTASE II



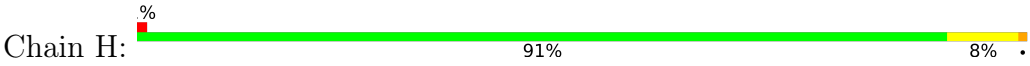


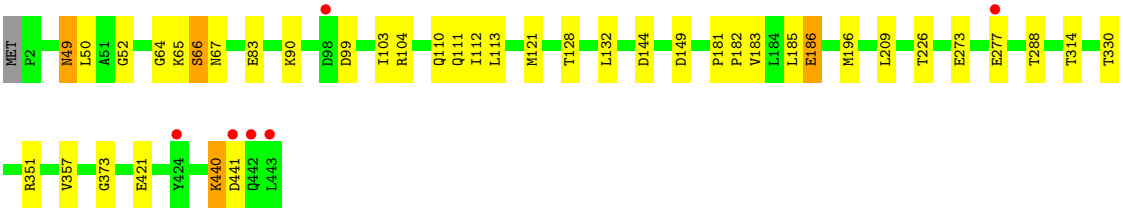
• Molecule 2: METHYL-COENZYME M REDUCTASE II



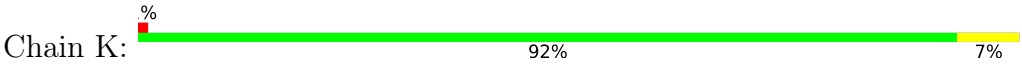


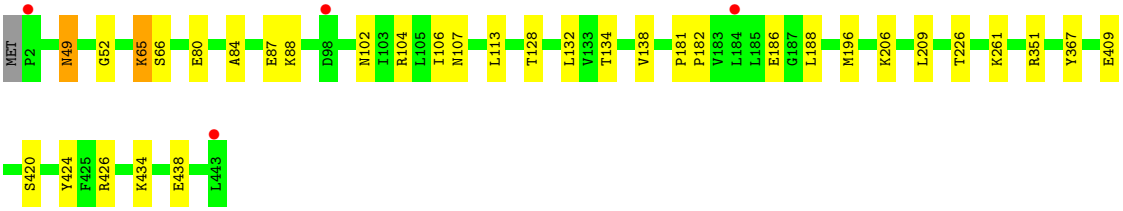
• Molecule 2: METHYL-COENZYME M REDUCTASE II



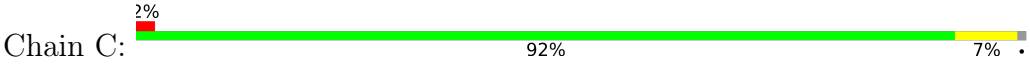


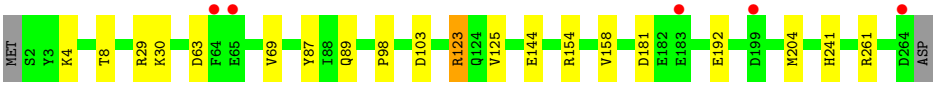
• Molecule 2: METHYL-COENZYME M REDUCTASE II



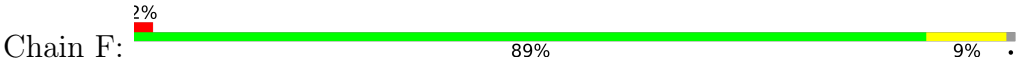


• Molecule 3: METHYL-COENZYME M REDUCTASE II

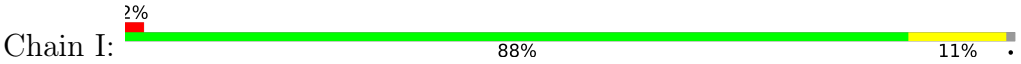


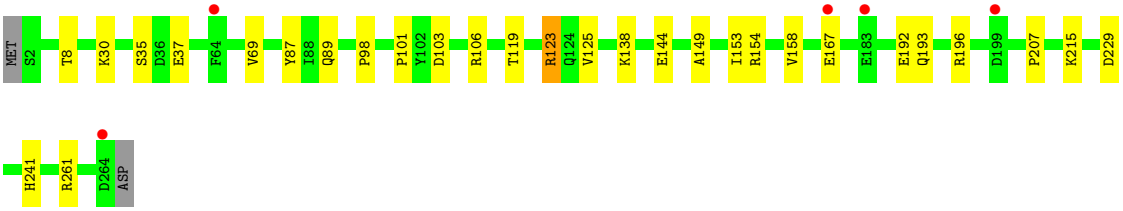


• Molecule 3: METHYL-COENZYME M REDUCTASE II

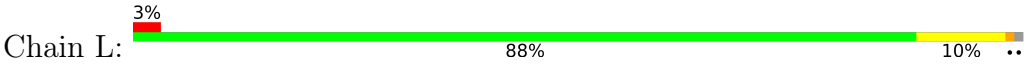


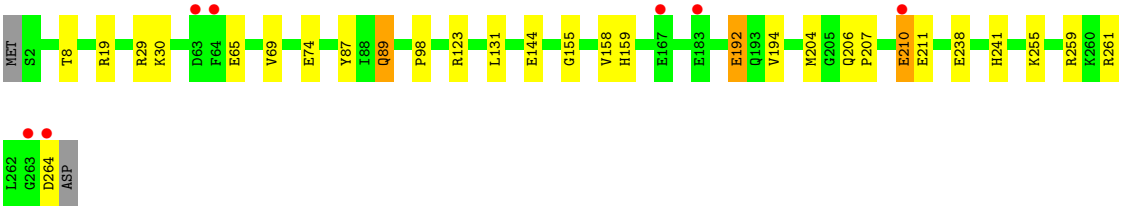
• Molecule 3: METHYL-COENZYME M REDUCTASE II





• Molecule 3: METHYL-COENZYME M REDUCTASE II





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	110.39Å 102.19Å 118.74Å 89.20° 93.97° 90.98°	Depositor
Resolution (Å)	48.66 – 1.80 48.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.66-1.80) 96.9 (48.66-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.165 , 0.201 0.166 , 0.200	Depositor DCC
R_{free} test set	23256 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.3	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.247 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	42336	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: TP7, MGN, MHS, GL3, SMC, ACT, NA, AGM, F43, 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	0.74	0/4336	0.83	8/5865 (0.1%)
1	D	0.76	0/4337	0.84	8/5870 (0.1%)
1	G	0.76	0/4335	0.80	5/5865 (0.1%)
1	J	0.77	0/4340	0.84	7/5874 (0.1%)
2	B	0.70	2/3378 (0.1%)	0.83	8/4589 (0.2%)
2	E	0.72	3/3385 (0.1%)	0.81	5/4598 (0.1%)
2	H	0.72	2/3394 (0.1%)	0.81	7/4610 (0.2%)
2	K	0.67	0/3427	0.77	1/4652 (0.0%)
3	C	0.73	0/2206	0.87	5/2974 (0.2%)
3	F	0.72	2/2192 (0.1%)	0.92	6/2955 (0.2%)
3	I	0.70	0/2192	0.83	3/2953 (0.1%)
3	L	0.73	0/2221	0.86	2/2993 (0.1%)
All	All	0.73	9/39743 (0.0%)	0.83	65/53798 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
2	B	0	1
3	F	0	1
3	L	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	66	SER	CB-OG	-10.73	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	277	GLU	CG-CD	6.59	1.61	1.51
2	E	277	GLU	CB-CG	-6.28	1.40	1.52
2	B	409	GLU	CB-CG	-6.25	1.40	1.52
2	B	186	GLU	CB-CG	-5.18	1.42	1.52

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	122	LYS	CD-CE-NZ	-13.94	79.65	111.70
1	J	190	LYS	CB-CG-CD	12.94	145.24	111.60
1	A	244	LYS	CD-CE-NZ	12.33	140.05	111.70
3	C	4	LYS	CB-CG-CD	-10.62	83.99	111.60
1	A	244	LYS	CB-CG-CD	-9.75	86.24	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	409	GLU	Sidechain
1	D	38	GLU	Sidechain
3	F	65	GLU	Sidechain
1	G	179	GLU	Sidechain
3	L	210	GLU	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	4273	0	4138	42	0
1	D	4276	0	4132	39	0
1	G	4271	0	4129	41	0
1	J	4273	0	4136	40	0
2	B	3315	0	3332	18	0
2	E	3319	0	3334	28	1
2	H	3325	0	3351	34	1
2	K	3348	0	3382	35	0
3	C	2155	0	2098	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2147	0	2090	17	1
3	I	2147	0	2096	23	0
3	L	2167	0	2123	28	1
4	A	7	0	5	1	0
4	D	7	0	5	0	0
4	G	7	0	4	1	0
4	J	7	0	5	1	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
5	J	42	0	38	0	0
6	A	4	0	3	0	0
6	D	4	0	3	0	0
6	E	8	0	6	1	0
6	F	4	0	3	0	0
6	G	4	0	3	0	0
6	H	4	0	3	0	0
6	I	4	0	3	0	0
6	J	4	0	3	0	0
6	K	4	0	3	0	0
6	L	4	0	3	0	0
7	D	124	0	86	6	0
7	G	62	0	43	2	0
7	J	62	0	43	1	0
8	F	1	0	0	0	0
9	A	381	0	0	12	0
9	B	281	0	0	6	0
9	C	152	0	0	4	1
9	D	284	0	0	7	0
9	E	223	0	0	5	0
9	F	145	0	0	2	0
9	G	385	0	0	7	0
9	H	269	0	0	8	0
9	I	147	0	0	5	0
9	J	291	0	0	6	0
9	K	224	0	0	8	0
9	L	133	0	0	4	1
All	All	42336	0	38641	310	3

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 4.

The worst 5 of 310 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:80:GLU:OE1	9:K:2043:HOH:O	1.63	1.16
3:I:89[B]:GLN:NE2	1:J:246:CYS:SG	2.19	1.13
3:C:89[B]:GLN:NE2	1:D:246[B]:CYS:SG	2.30	1.05
9:C:2070:HOH:O	1:D:246[B]:CYS:SG	2.19	0.99
2:H:83:GLU:OE1	9:H:2063:HOH:O	1.81	0.99

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:GLU:OE2	9:L:2032:HOH:O[1_445]	1.77	0.43
2:H:110:GLN:NE2	9:C:2024:HOH:O[1_564]	2.14	0.06
3:F:65:GLU:OE2	3:L:211:GLU:OE1[1_445]	2.16	0.04

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	549/554 (99%)	531 (97%)	15 (3%)	3 (0%)	29	15
1	D	549/554 (99%)	534 (97%)	14 (3%)	1 (0%)	47	33
1	G	549/554 (99%)	531 (97%)	17 (3%)	1 (0%)	47	33
1	J	549/554 (99%)	531 (97%)	17 (3%)	1 (0%)	47	33
2	B	443/443 (100%)	438 (99%)	5 (1%)	0	100	100
2	E	444/443 (100%)	440 (99%)	3 (1%)	1 (0%)	47	33
2	H	445/443 (100%)	440 (99%)	5 (1%)	0	100	100
2	K	448/443 (101%)	444 (99%)	4 (1%)	0	100	100
3	C	265/265 (100%)	259 (98%)	6 (2%)	0	100	100
3	F	263/265 (99%)	257 (98%)	6 (2%)	0	100	100
3	I	263/265 (99%)	256 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	L	266/265 (100%)	259 (97%)	7 (3%)	0	100 100
All	All	5033/5048 (100%)	4920 (98%)	106 (2%)	7 (0%)	51 36

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	SER
1	D	465	SER
1	G	465	SER
1	J	465	SER
2	E	65	LYS

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	440/438 (100%)	436 (99%)	4 (1%)	78 75
1	D	440/438 (100%)	437 (99%)	3 (1%)	84 81
1	G	440/438 (100%)	436 (99%)	4 (1%)	78 75
1	J	441/438 (101%)	438 (99%)	3 (1%)	84 81
2	B	348/346 (101%)	346 (99%)	2 (1%)	86 84
2	E	349/346 (101%)	348 (100%)	1 (0%)	92 91
2	H	350/346 (101%)	348 (99%)	2 (1%)	86 84
2	K	353/346 (102%)	349 (99%)	4 (1%)	73 68
3	C	234/232 (101%)	230 (98%)	4 (2%)	60 51
3	F	232/232 (100%)	229 (99%)	3 (1%)	69 62
3	I	232/232 (100%)	226 (97%)	6 (3%)	46 32
3	L	235/232 (101%)	230 (98%)	5 (2%)	53 42
All	All	4094/4064 (101%)	4053 (99%)	41 (1%)	78 71

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	261	ARG
2	K	424[B]	TYR
1	J	347	ASP
2	K	49	ASN
3	L	89[A]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	134	ASN
2	K	111	GLN
2	H	49	ASN
3	L	77	GLN
2	K	49	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

20 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	SMC	D	455	1	5,6,7	1.03	0	2,6,8	0.88	0
1	MHS	D	261	1	7,11,12	1.21	1 (14%)	6,14,16	1.59	2 (33%)
1	AGM	D	275	1	10,11,12	2.62	3 (30%)	6,13,15	2.70	3 (50%)
1	SMC	A	455	1	5,6,7	1.14	0	2,6,8	1.31	0
1	MHS	A	261	1	7,11,12	1.21	0	6,14,16	2.23	4 (66%)
1	MGN	D	403	1	6,9,10	1.10	1 (16%)	5,12,14	0.66	0
1	SMC	J	455	1	5,6,7	0.93	0	2,6,8	1.22	0
1	SMC	G	455	1	5,6,7	0.96	0	2,6,8	1.87	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GL3	D	448	1	2,3,4	3.16	1 (50%)	1,2,4	0.07	0
1	MGN	A	403	1	6,9,10	0.90	0	5,12,14	0.80	0
1	MHS	G	261	1	7,11,12	1.07	0	6,14,16	1.60	2 (33%)
1	MGN	J	403	1	6,9,10	0.90	0	5,12,14	0.54	0
1	MHS	J	261	1	7,11,12	1.02	0	6,14,16	1.76	2 (33%)
1	GL3	G	448	1	2,3,4	4.52	1 (50%)	1,2,4	0.10	0
1	GL3	J	448	1	2,3,4	3.81	1 (50%)	1,2,4	0.11	0
1	GL3	A	448	1	2,3,4	4.43	1 (50%)	1,2,4	0.03	0
1	AGM	G	275	1	10,11,12	2.63	3 (30%)	6,13,15	3.08	4 (66%)
1	AGM	J	275	1	10,11,12	2.22	3 (30%)	6,13,15	3.24	4 (66%)
1	AGM	A	275	1	10,11,12	2.34	3 (30%)	6,13,15	3.01	4 (66%)
1	MGN	G	403	1	6,9,10	0.95	0	5,12,14	0.59	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	SMC	D	455	1	-	1/3/5/7	-
1	MHS	D	261	1	-	0/5/6/8	0/1/1/1
1	AGM	D	275	1	-	2/10/11/13	-
1	SMC	A	455	1	-	1/3/5/7	-
1	MHS	A	261	1	-	0/5/6/8	0/1/1/1
1	MGN	D	403	1	-	0/7/9/12	-
1	SMC	J	455	1	-	1/3/5/7	-
1	SMC	G	455	1	-	0/3/5/7	-
1	GL3	D	448	1	-	0/1/1/2	-
1	MGN	A	403	1	-	0/7/9/12	-
1	MHS	G	261	1	-	0/5/6/8	0/1/1/1
1	MGN	J	403	1	-	0/7/9/12	-
1	MHS	J	261	1	-	0/5/6/8	0/1/1/1
1	GL3	G	448	1	-	0/1/1/2	-
1	GL3	J	448	1	-	0/1/1/2	-
1	GL3	A	448	1	-	1/1/1/2	-
1	AGM	G	275	1	-	3/10/11/13	-
1	AGM	J	275	1	-	4/10/11/13	-
1	AGM	A	275	1	-	3/10/11/13	-
1	MGN	G	403	1	-	0/7/9/12	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	275	AGM	CZ-NE1	6.84	1.45	1.33
1	G	275	AGM	CZ-NE1	6.71	1.44	1.33
1	G	448	GL3	C-S	-6.39	1.58	1.80
1	A	448	GL3	C-S	-6.27	1.59	1.80
1	A	275	AGM	CZ-NE1	5.86	1.43	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	275	AGM	NH1-CZ-NE1	-5.32	107.66	119.55
1	G	275	AGM	NH1-CZ-NE1	-5.30	107.70	119.55
1	A	275	AGM	NH1-CZ-NE1	-5.10	108.15	119.55
1	D	275	AGM	NH1-CZ-NE1	-5.10	108.16	119.55
1	J	275	AGM	NE1-CZ-NH2	-4.03	113.55	120.59

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	275	AGM	CE2-CD-CG-CB
1	A	275	AGM	NH2-CZ-NE1-CD
1	G	275	AGM	CE2-CD-CG-CB
1	G	275	AGM	NH2-CZ-NE1-CD
1	J	275	AGM	CE2-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	455	SMC	1	0
1	A	455	SMC	1	0
1	G	448	GL3	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ACT	E	1444	-	3,3,3	0.72	0	3,3,3	1.56	1 (33%)
4	COM	G	1553	7	6,6,6	1.94	2 (33%)	7,8,8	4.28	4 (57%)
7	F43	G	1554	4,1	61,71,71	2.20	10 (16%)	64,118,118	1.61	13 (20%)
5	TP7	J	1553	-	19,20,20	0.91	1 (5%)	24,26,26	1.11	3 (12%)
6	ACT	D	1557	-	3,3,3	0.88	0	3,3,3	1.12	0
6	ACT	A	1555	-	3,3,3	0.52	0	3,3,3	1.66	1 (33%)
7	F43	J	1554	4,1	61,71,71	2.43	9 (14%)	64,118,118	1.44	10 (15%)
4	COM	A	1553	7	6,6,6	1.71	2 (33%)	7,8,8	4.55	4 (57%)
5	TP7	A	1554	-	19,20,20	1.14	1 (5%)	24,26,26	0.99	1 (4%)
6	ACT	H	1444	-	3,3,3	0.65	0	3,3,3	1.62	1 (33%)
7	F43	D	1556	4,1	61,71,71	2.20	10 (16%)	64,118,118	1.55	12 (18%)
5	TP7	J	1556	-	19,20,20	0.86	1 (5%)	24,26,26	1.09	0
4	COM	D	1555	7	6,6,6	2.04	2 (33%)	7,8,8	3.57	3 (42%)
6	ACT	G	1555	-	3,3,3	1.09	0	3,3,3	1.43	0
7	F43	D	1554	4,1	61,71,71	2.38	11 (18%)	64,118,118	1.71	13 (20%)
6	ACT	J	1557	-	3,3,3	0.61	0	3,3,3	1.45	0
4	COM	J	1555	7	6,6,6	1.55	2 (33%)	7,8,8	3.09	3 (42%)
6	ACT	E	1445	-	3,3,3	0.70	0	3,3,3	1.53	1 (33%)
6	ACT	I	1265	-	3,3,3	0.73	0	3,3,3	1.12	0
6	ACT	L	1265	-	3,3,3	0.78	0	3,3,3	1.12	0
6	ACT	K	1444	-	3,3,3	0.83	0	3,3,3	0.89	0
5	TP7	D	1553	-	19,20,20	1.15	2 (10%)	24,26,26	1.36	5 (20%)
6	ACT	F	1265	-	3,3,3	0.65	0	3,3,3	1.25	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
4	COM	G	1553	7	-	0/4/4/4	-
7	F43	G	1554	4,1	-	5/28/185/185	-
5	TP7	J	1553	-	-	2/24/24/24	-
7	F43	D	1554	4,1	-	7/28/185/185	-
7	F43	J	1554	4,1	-	5/28/185/185	-
4	COM	J	1555	7	-	4/4/4/4	-
5	TP7	D	1553	-	-	1/24/24/24	-
7	F43	D	1556	4,1	-	5/28/185/185	-
4	COM	A	1553	7	-	0/4/4/4	-
5	TP7	A	1554	-	-	1/24/24/24	-
5	TP7	J	1556	-	-	2/24/24/24	-
4	COM	D	1555	7	-	0/4/4/4	-

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1556	F43	NI-NA	10.28	2.11	1.89
7	J	1554	F43	NI-NA	9.72	2.10	1.89
7	D	1554	F43	NI-NA	9.60	2.10	1.89
7	D	1554	F43	NI-NB	9.16	2.09	1.89
7	J	1554	F43	NI-NB	8.49	2.07	1.89

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1553	COM	O2S-S2-C2	8.99	117.74	106.92
4	A	1553	COM	O2S-S2-C2	8.87	117.60	106.92
4	A	1553	COM	O3S-S2-O2S	-6.62	95.11	111.27
4	D	1555	COM	O2S-S2-C2	6.54	114.80	106.92
4	J	1555	COM	O2S-S2-C2	5.31	113.31	106.92

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1555	COM	S1-C1-C2-S2
4	J	1555	COM	C1-C2-S2-O1S
4	J	1555	COM	C1-C2-S2-O2S
4	J	1555	COM	C1-C2-S2-O3S
5	D	1553	TP7	CB-O4P-P-O2P

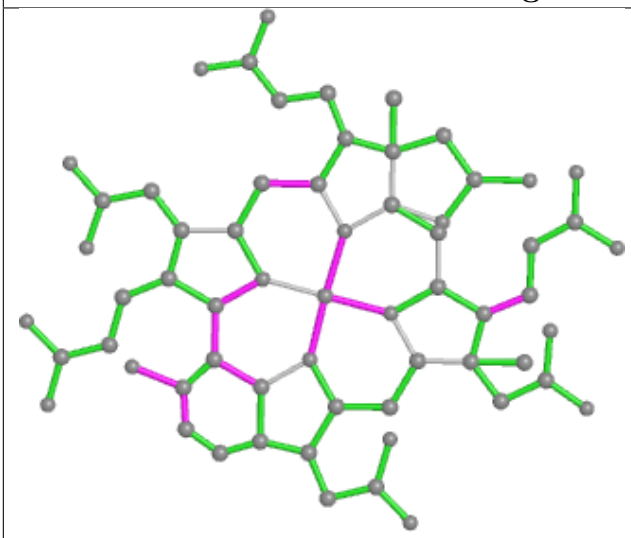
There are no ring outliers.

8 monomers are involved in 13 short contacts:

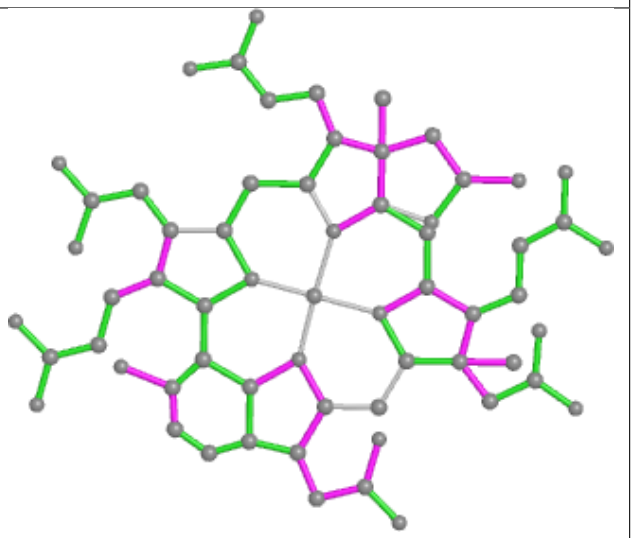
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1553	COM	1	0
7	G	1554	F43	2	0
7	J	1554	F43	1	0
4	A	1553	COM	1	0
7	D	1556	F43	3	0
7	D	1554	F43	3	0
4	J	1555	COM	1	0
6	E	1445	ACT	1	0

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.

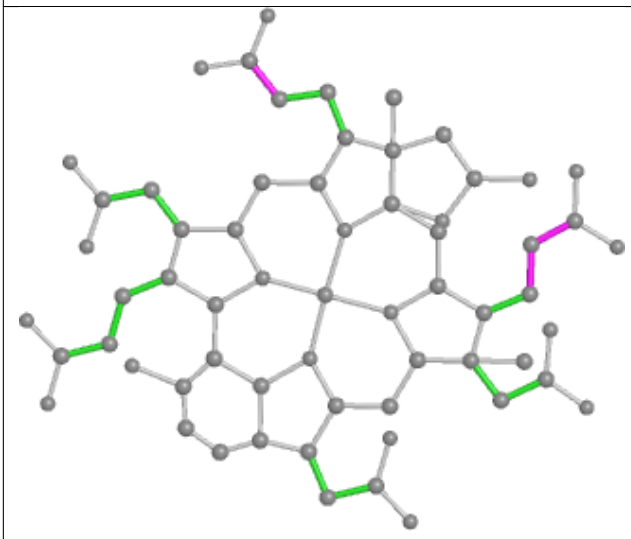
Ligand F43 G 1554



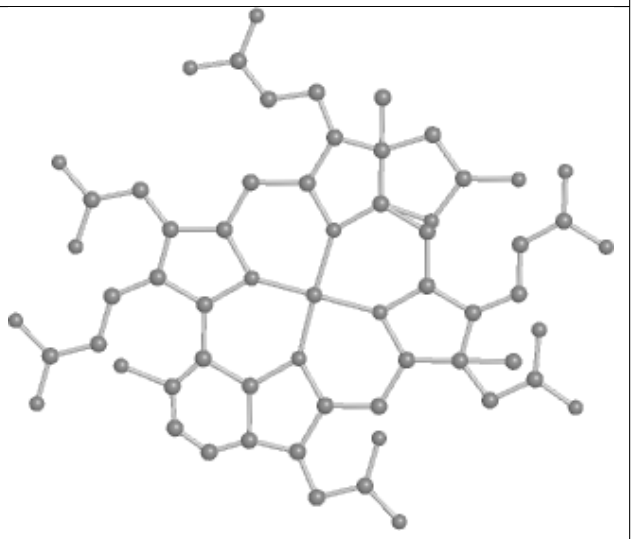
Bond lengths



Bond angles

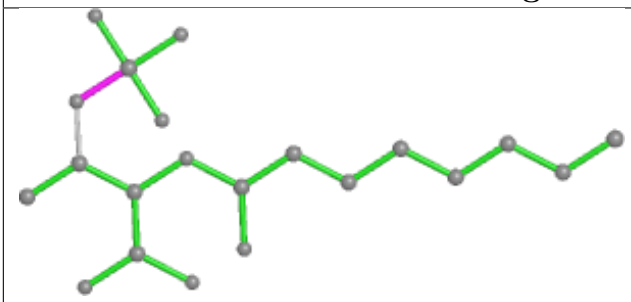


Torsions

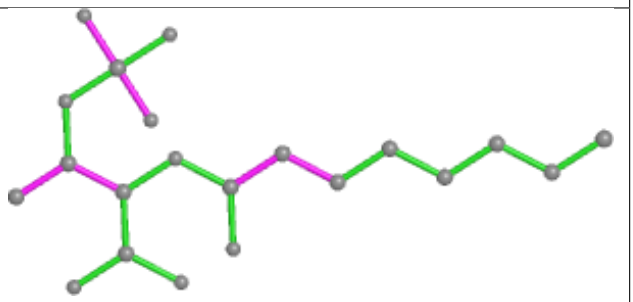


Rings

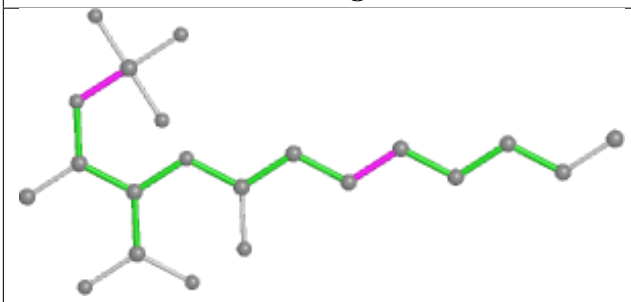
Ligand TP7 J 1553



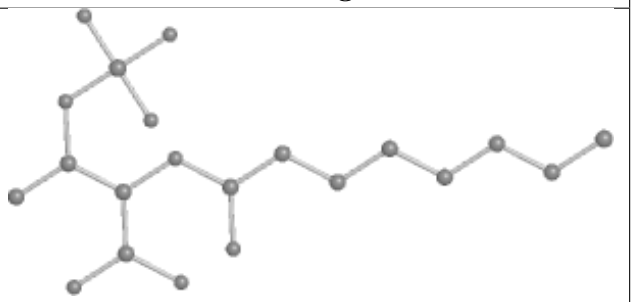
Bond lengths



Bond angles

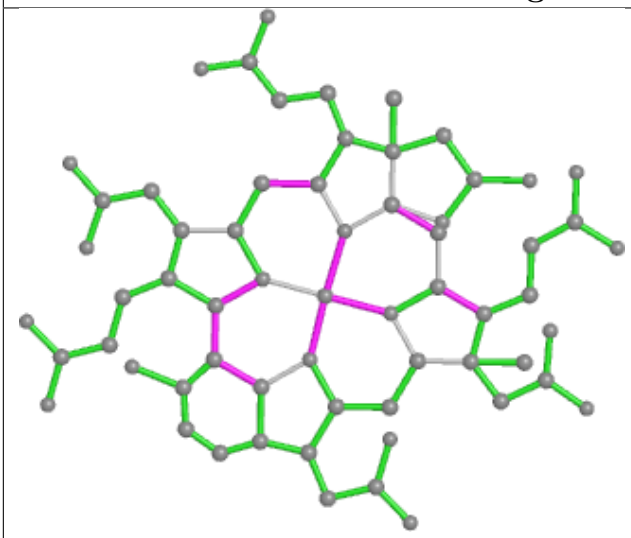


Torsions

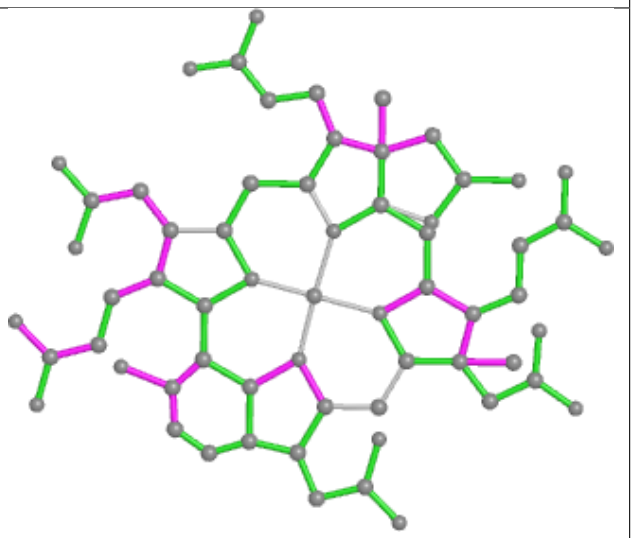


Rings

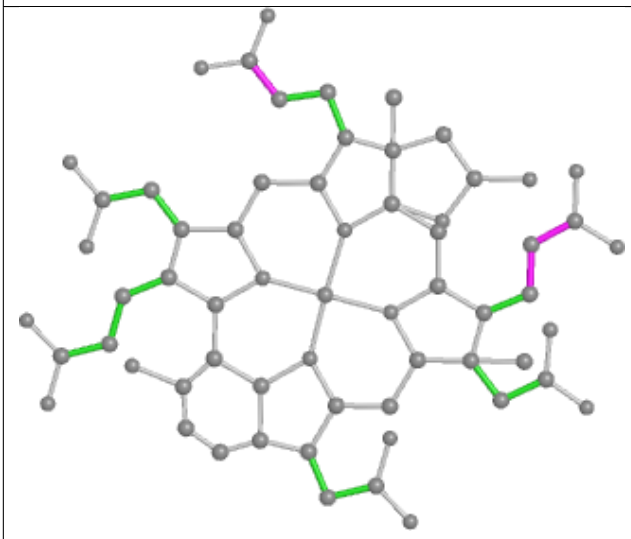
Ligand F43 J 1554



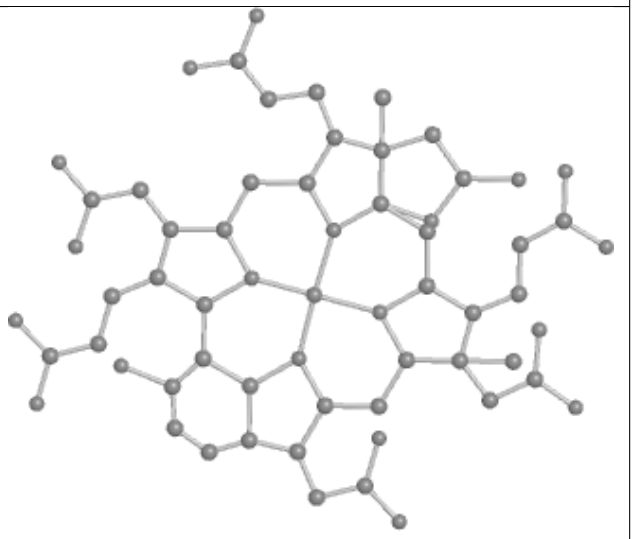
Bond lengths



Bond angles

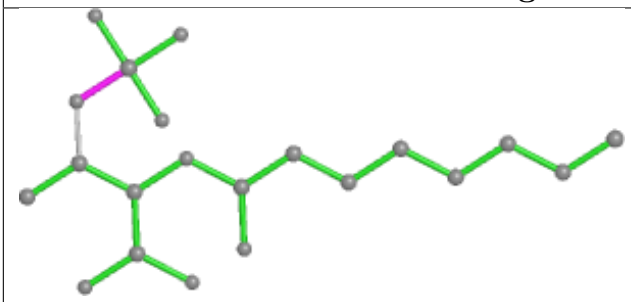


Torsions

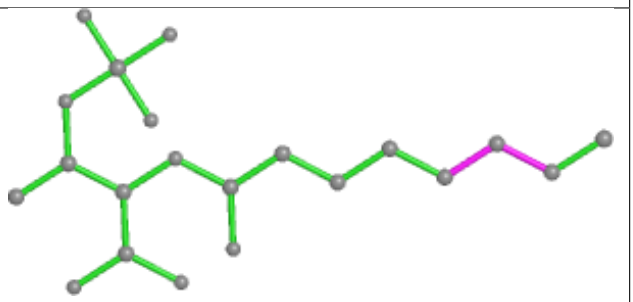


Rings

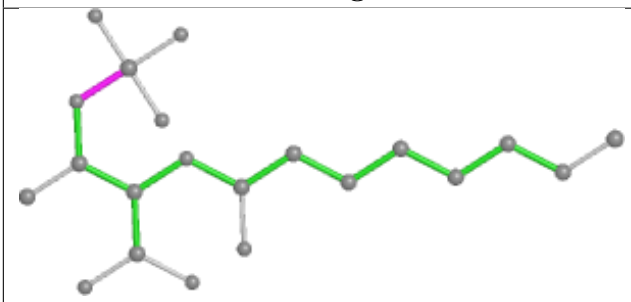
Ligand TP7 A 1554



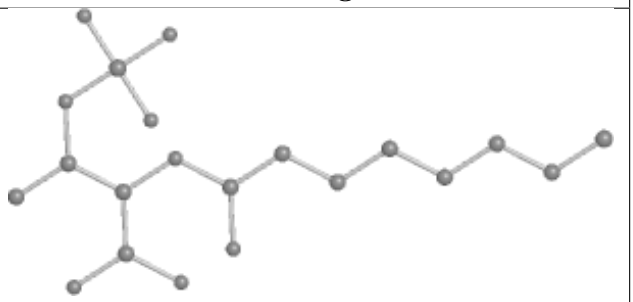
Bond lengths



Bond angles

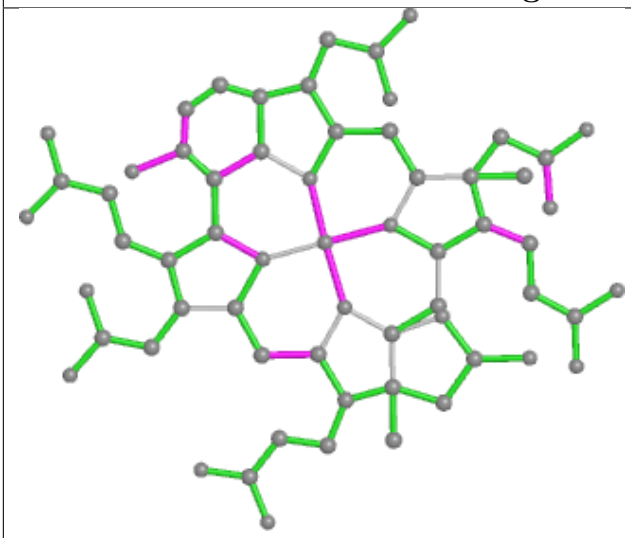


Torsions

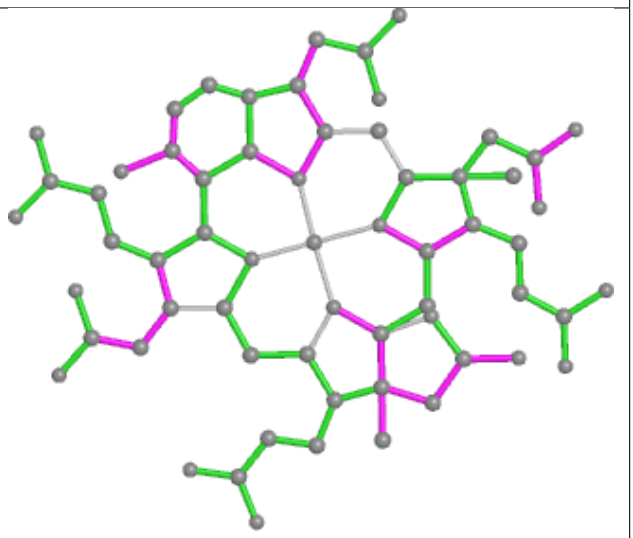


Rings

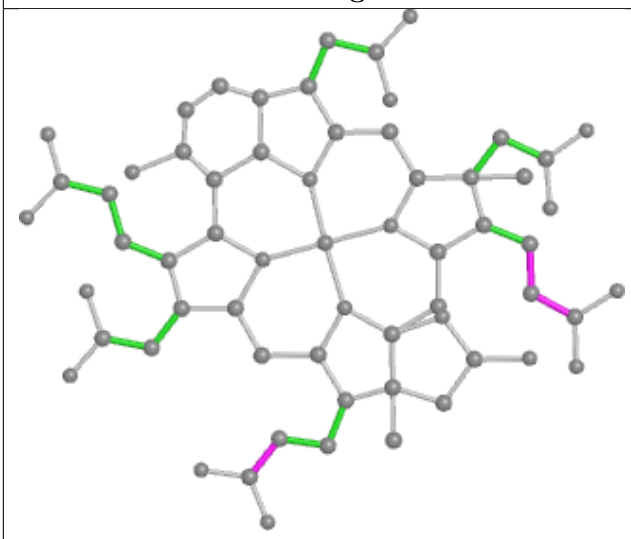
Ligand F43 D 1556



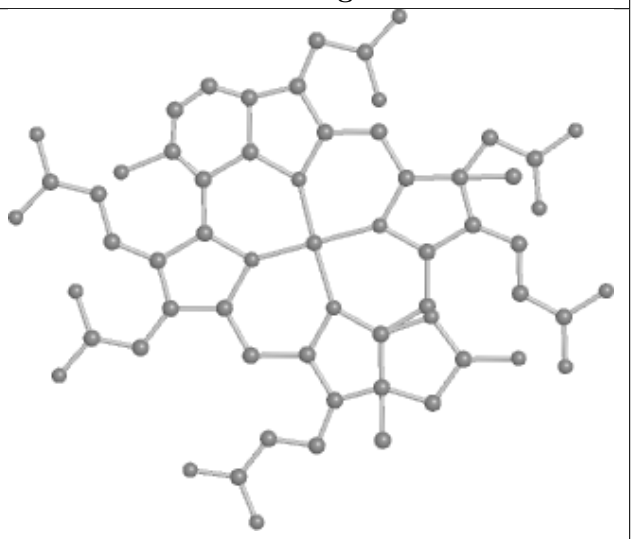
Bond lengths



Bond angles

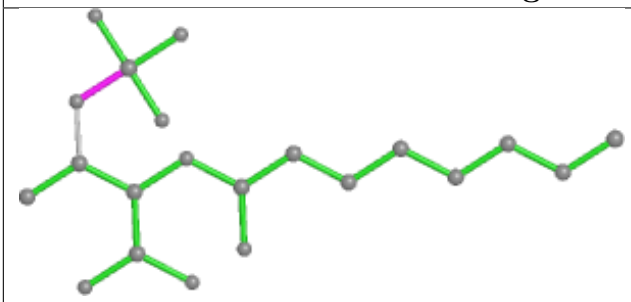


Torsions



Rings

Ligand TP7 J 1556



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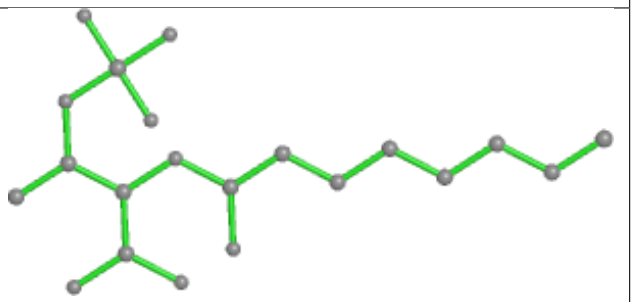
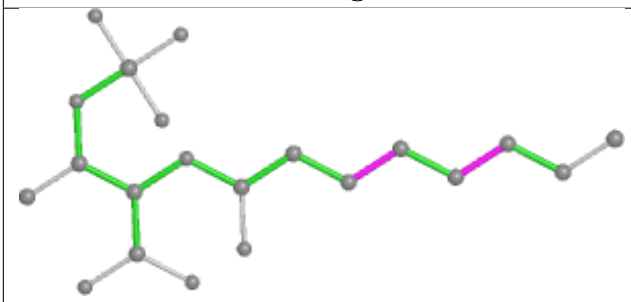


Bond angles



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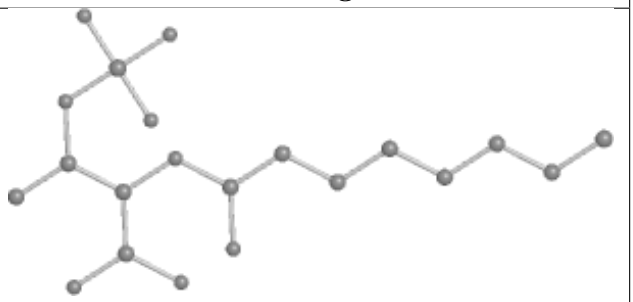
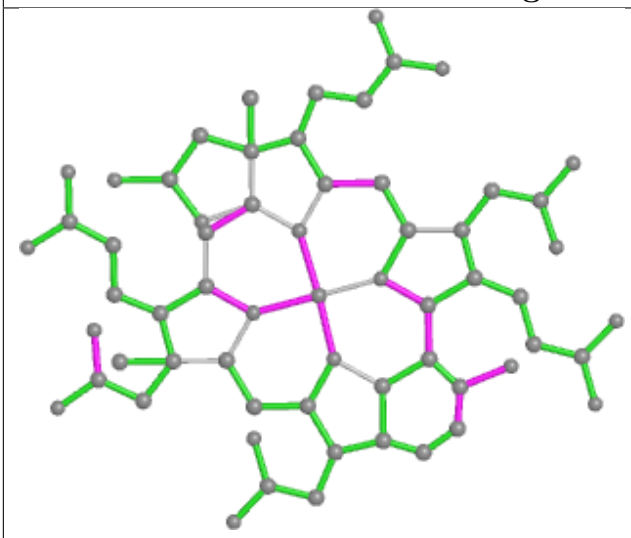


Rings

Ligand F43 D 1554



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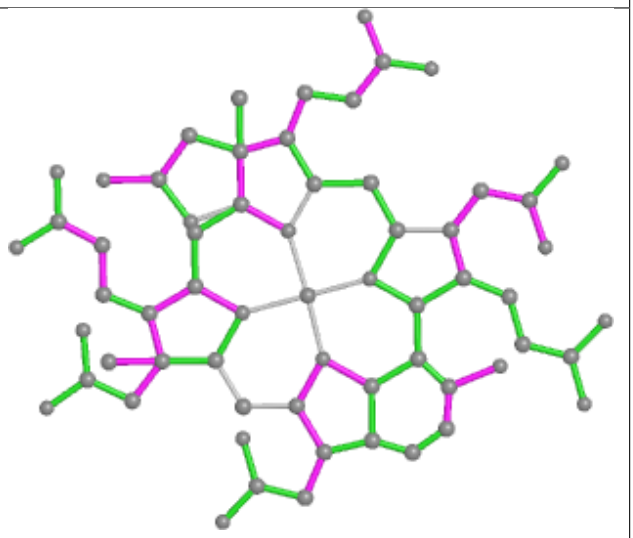
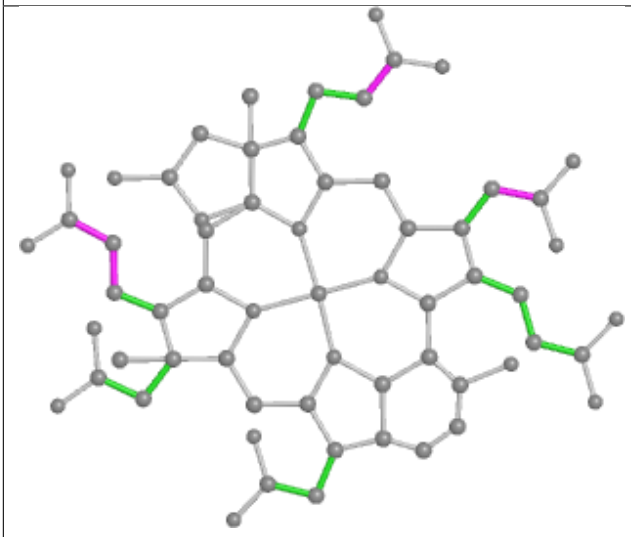
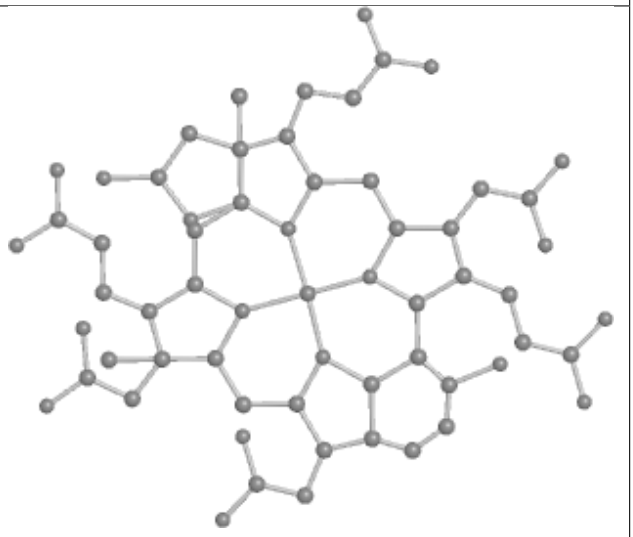


Bond angles

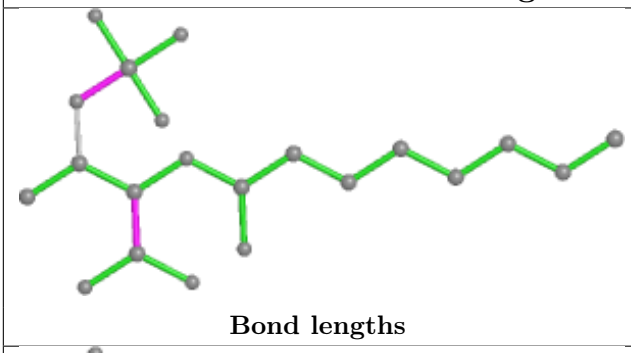


Torsions

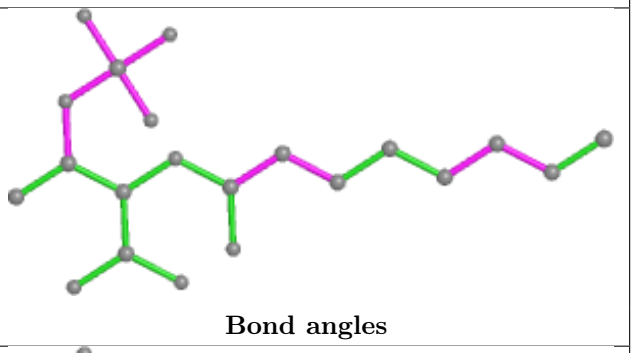


Rings

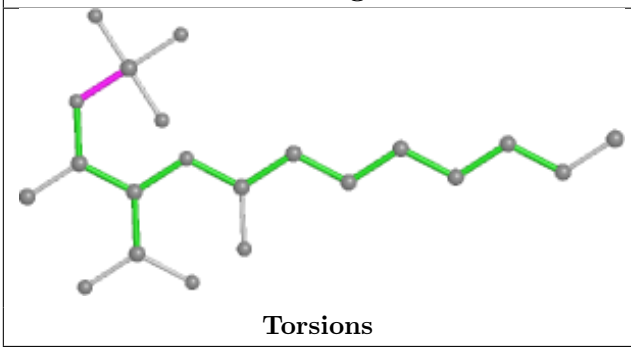
Ligand TP7 D 1553



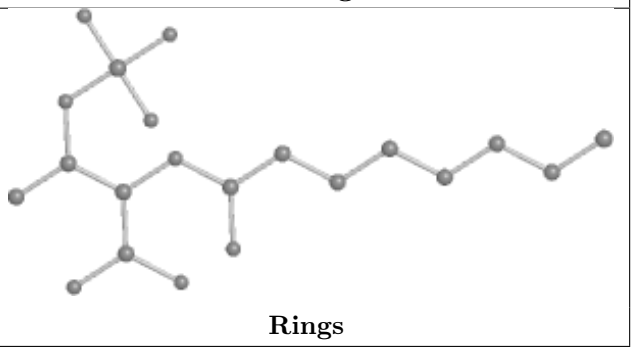
Bond lengths



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	543/554 (98%)	-0.03	5 (0%)	84	82	9, 14, 30, 44	1 (0%)
1	D	544/554 (98%)	-0.06	6 (1%)	80	78	8, 15, 30, 59	0
1	G	543/554 (98%)	-0.06	2 (0%)	92	90	8, 14, 29, 42	0
1	J	543/554 (98%)	-0.07	5 (0%)	84	82	9, 15, 30, 43	0
2	B	442/443 (99%)	-0.03	7 (1%)	72	68	9, 15, 29, 52	0
2	E	442/443 (99%)	-0.03	5 (1%)	80	78	9, 15, 29, 56	1 (0%)
2	H	442/443 (99%)	0.01	6 (1%)	75	72	10, 15, 29, 56	0
2	K	442/443 (99%)	0.02	4 (0%)	84	82	10, 15, 30, 52	0
3	C	263/265 (99%)	-0.00	5 (1%)	66	63	9, 17, 35, 66	0
3	F	263/265 (99%)	-0.05	5 (1%)	66	63	9, 16, 34, 56	0
3	I	263/265 (99%)	-0.07	5 (1%)	66	63	9, 17, 35, 59	0
3	L	263/265 (99%)	0.01	7 (2%)	54	49	9, 17, 35, 62	0
All	All	4993/5048 (98%)	-0.03	62 (1%)	79	76	8, 15, 31, 66	2 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	552	ALA	7.5
3	L	64	PHE	7.3
3	F	64	PHE	6.0
3	C	64	PHE	5.9
3	I	64	PHE	4.7

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

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	AGM	J	275	12/13	0.93	0.15	6,13,18,18	0
1	AGM	D	275	12/13	0.94	0.14	8,11,14,18	0
1	MHS	G	261	11/12	0.94	0.11	11,16,22,23	0
1	AGM	G	275	12/13	0.94	0.15	10,13,14,14	0
1	MHS	D	261	11/12	0.94	0.10	15,17,20,20	0
1	AGM	A	275	12/13	0.95	0.15	8,10,14,16	0
1	MHS	J	261	11/12	0.95	0.11	11,16,21,24	0
1	MHS	A	261	11/12	0.95	0.09	13,17,21,21	0
1	MGN	A	403	10/11	0.97	0.12	7,8,12,13	0
1	MGN	G	403	10/11	0.97	0.11	7,8,11,12	0
1	SMC	J	455	7/8	0.97	0.14	12,12,14,15	0
1	SMC	G	455	7/8	0.98	0.12	9,10,14,14	0
1	SMC	A	455	7/8	0.98	0.13	10,13,16,17	0
1	MGN	D	403	10/11	0.98	0.10	6,9,12,12	0
1	MGN	J	403	10/11	0.98	0.12	7,9,11,13	0
1	SMC	D	455	7/8	0.98	0.14	11,13,13,13	0
1	GL3	G	448	4/5	0.99	0.10	8,9,11,13	0
1	GL3	A	448	4/5	0.99	0.11	9,10,10,13	0
1	GL3	J	448	4/5	0.99	0.10	8,10,10,11	0
1	GL3	D	448	4/5	0.99	0.08	6,7,10,11	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
6	ACT	G	1555	4/4	0.67	0.24	30,32,35,35	0
6	ACT	E	1444	4/4	0.69	0.21	48,51,52,52	0
6	ACT	E	1445	4/4	0.76	0.21	39,41,43,47	0
6	ACT	F	1265	4/4	0.80	0.18	27,33,34,34	0
6	ACT	A	1555	4/4	0.80	0.20	34,37,38,39	0
6	ACT	K	1444	4/4	0.81	0.21	44,46,47,48	0

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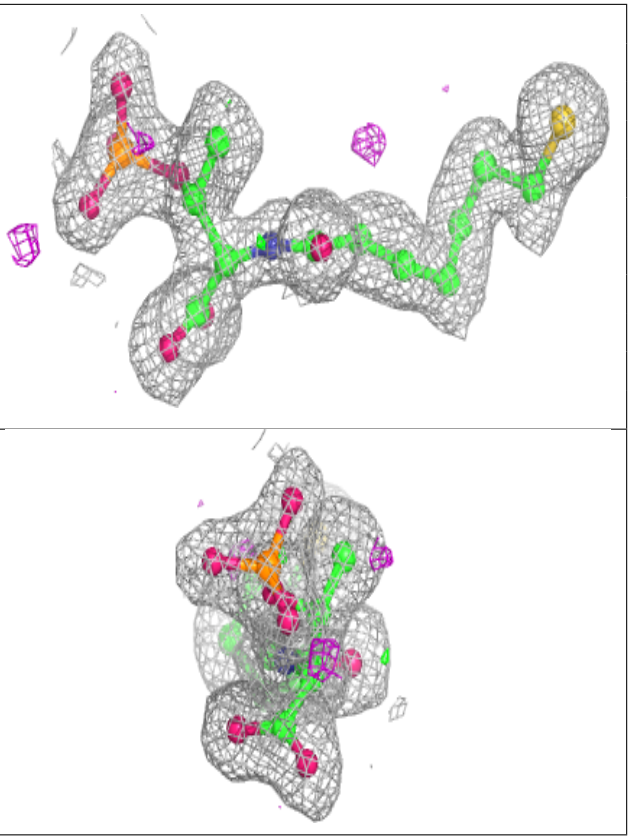
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	L	1265	4/4	0.81	0.19	31,37,37,39	0
6	ACT	H	1444	4/4	0.84	0.27	35,36,38,42	0
6	ACT	I	1265	4/4	0.88	0.13	31,38,38,38	0
6	ACT	D	1557	4/4	0.90	0.19	38,39,40,41	0
6	ACT	J	1557	4/4	0.91	0.19	35,39,41,42	0
4	COM	D	1555	7/7	0.94	0.19	4,10,13,20	7
5	TP7	J	1553	21/21	0.95	0.12	9,14,20,21	0
4	COM	A	1553	7/7	0.95	0.19	8,13,18,20	7
4	COM	G	1553	7/7	0.95	0.21	5,9,14,17	7
4	COM	J	1555	7/7	0.95	0.16	8,11,18,23	7
8	NA	F	1270	1/1	0.95	0.09	37,37,37,37	0
5	TP7	D	1553	21/21	0.96	0.12	10,15,18,20	0
5	TP7	A	1554	21/21	0.96	0.13	9,15,21,21	0
5	TP7	J	1556	21/21	0.96	0.11	10,15,20,20	0
7	F43	D	1556	62/62	0.97	0.13	3,10,17,19	0
7	F43	G	1554	62/62	0.97	0.11	4,10,16,18	0
7	F43	J	1554	62/62	0.97	0.11	3,11,16,19	0
7	F43	D	1554	62/62	0.97	0.11	1,9,16,18	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.

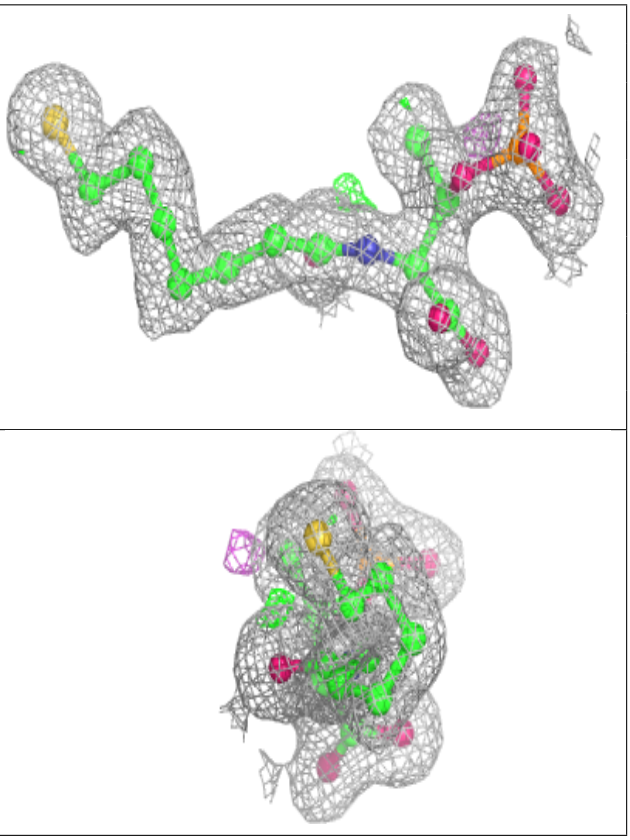
Electron density around TP7 J 1553:

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



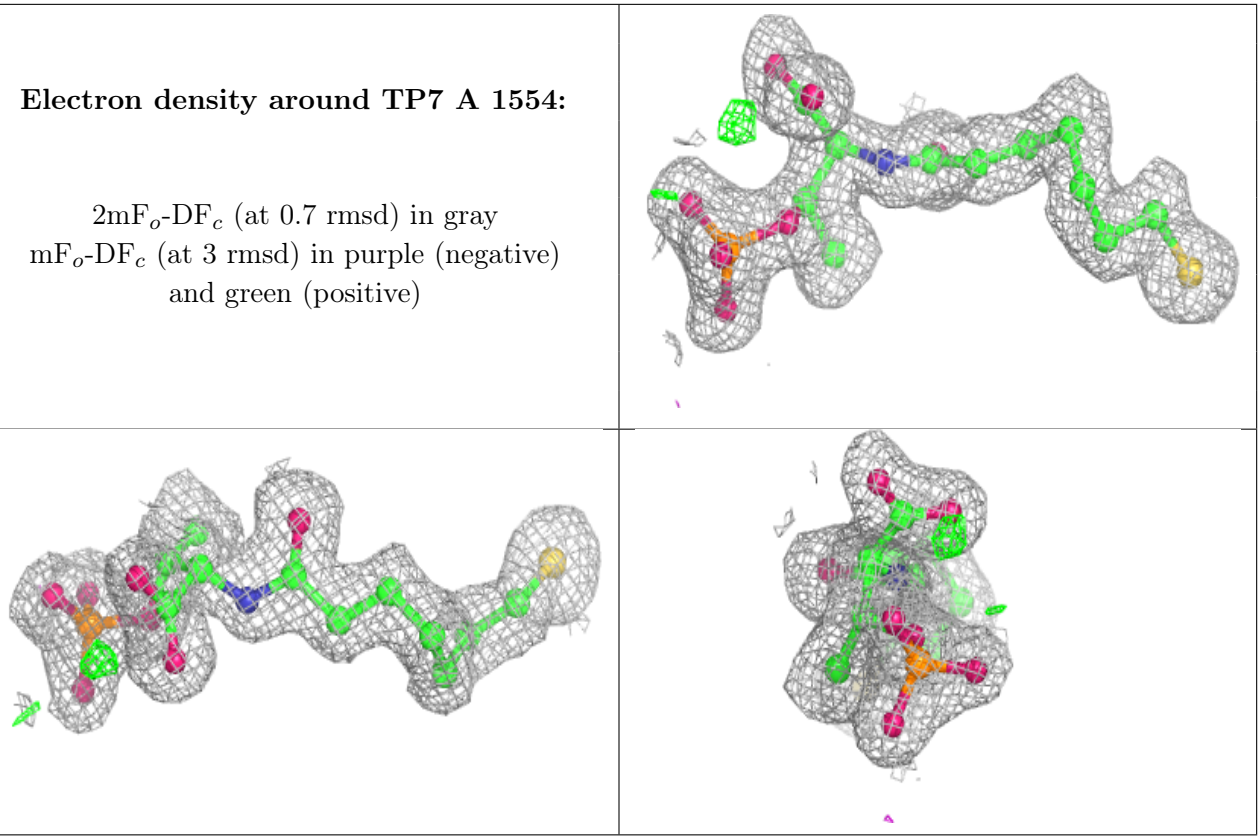
Electron density around TP7 D 1553:

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



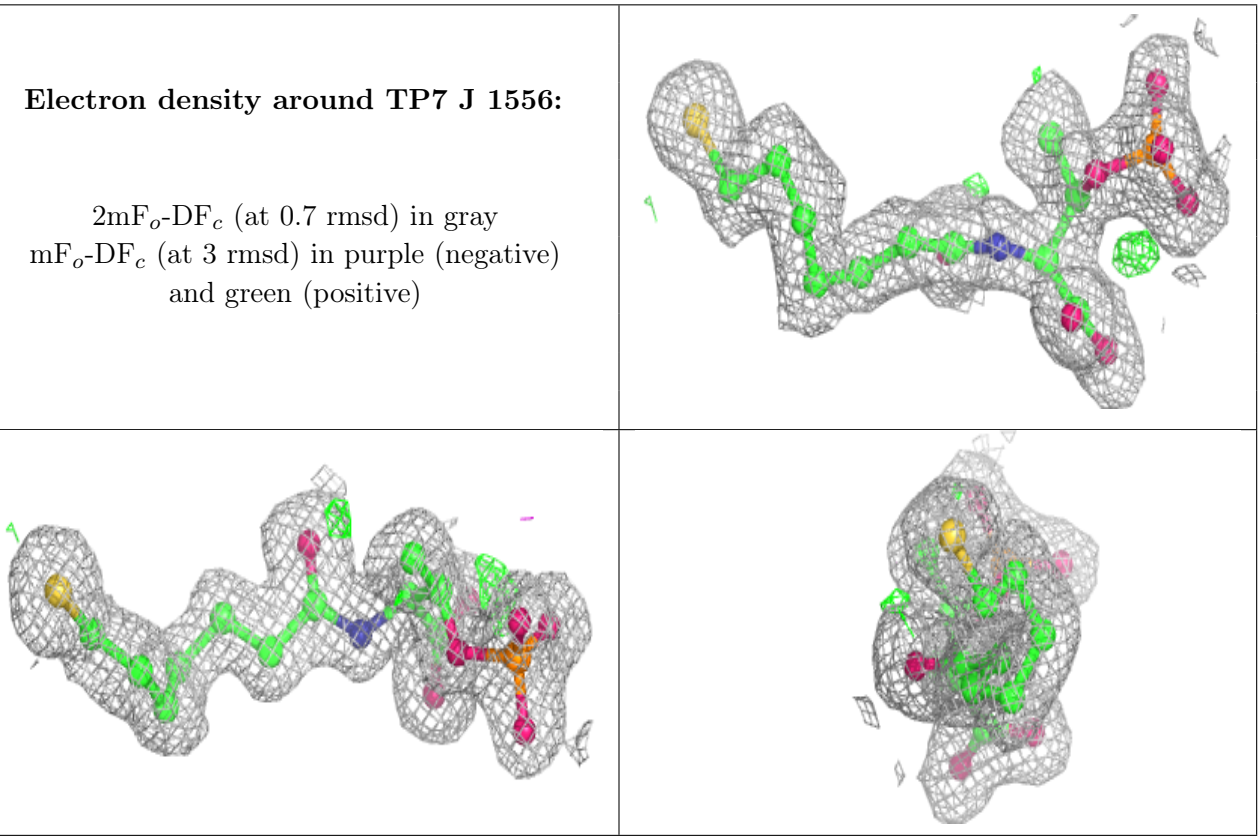
Electron density around TP7 A 1554:

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



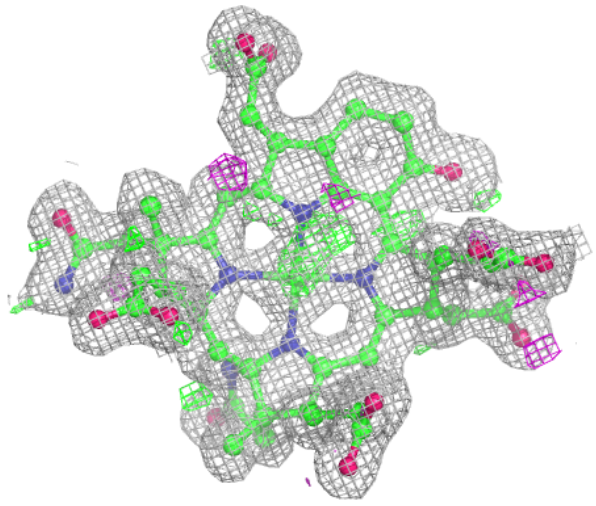
Electron density around TP7 J 1556:

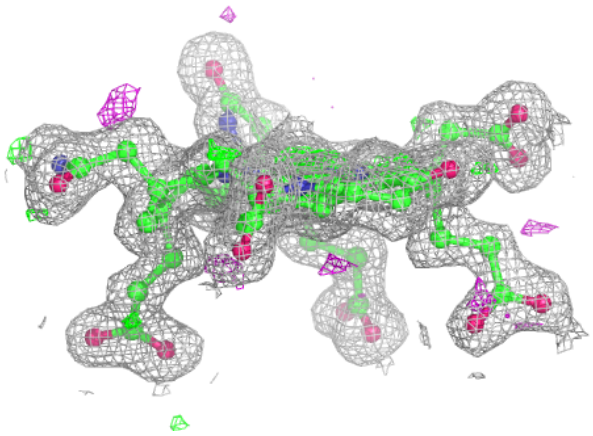
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

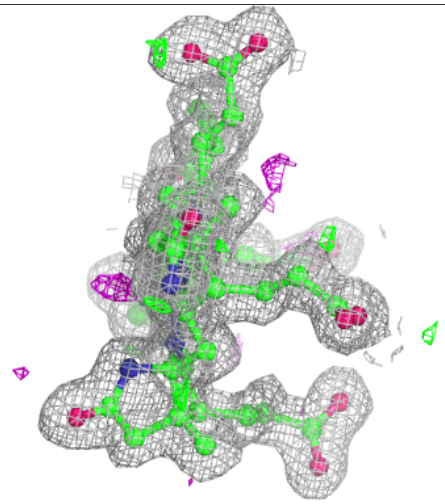


Electron density around F43 D 1556:

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

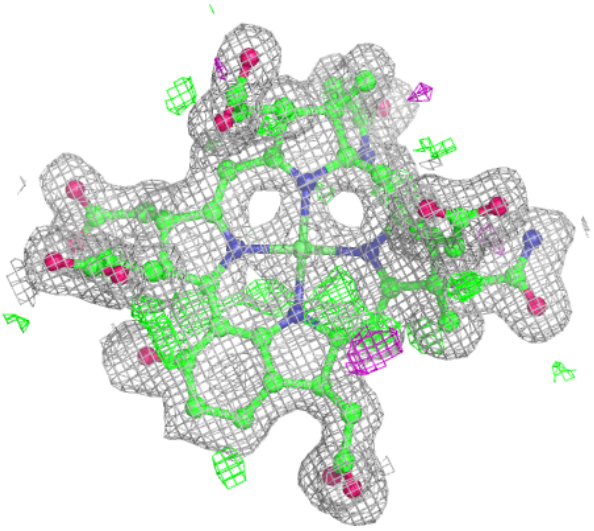


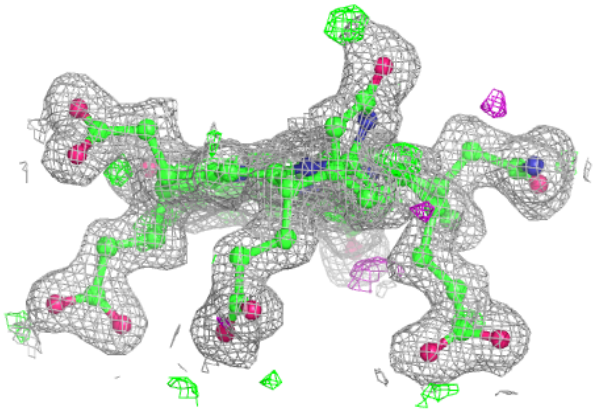


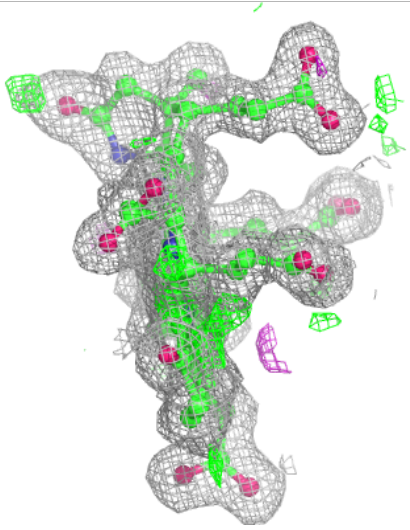


Electron density around F43 G 1554:

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

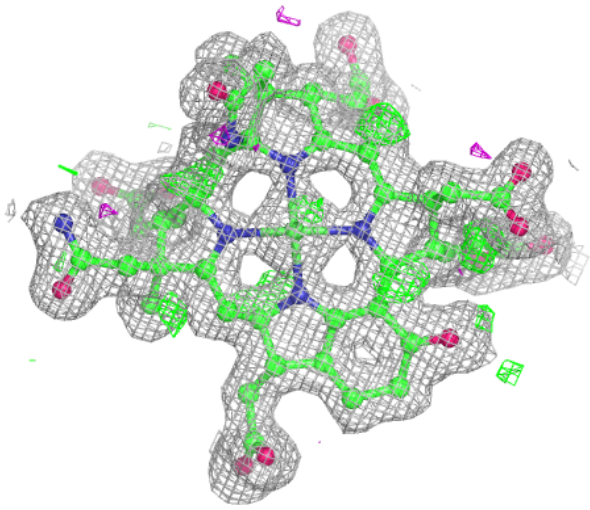


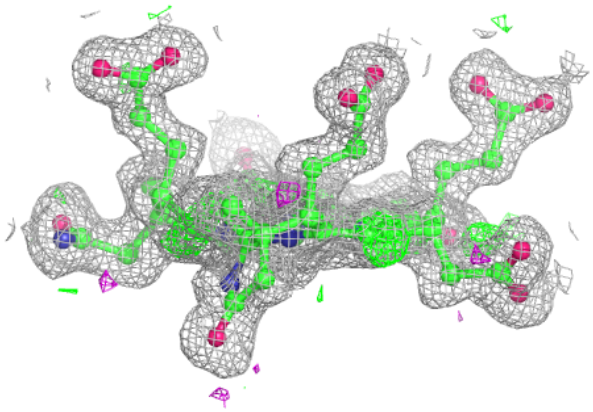


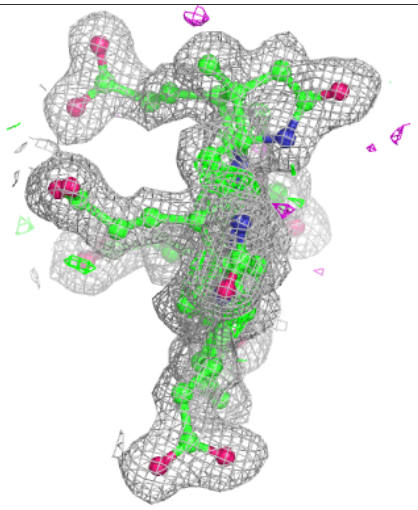


Electron density around F43 J 1554:

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

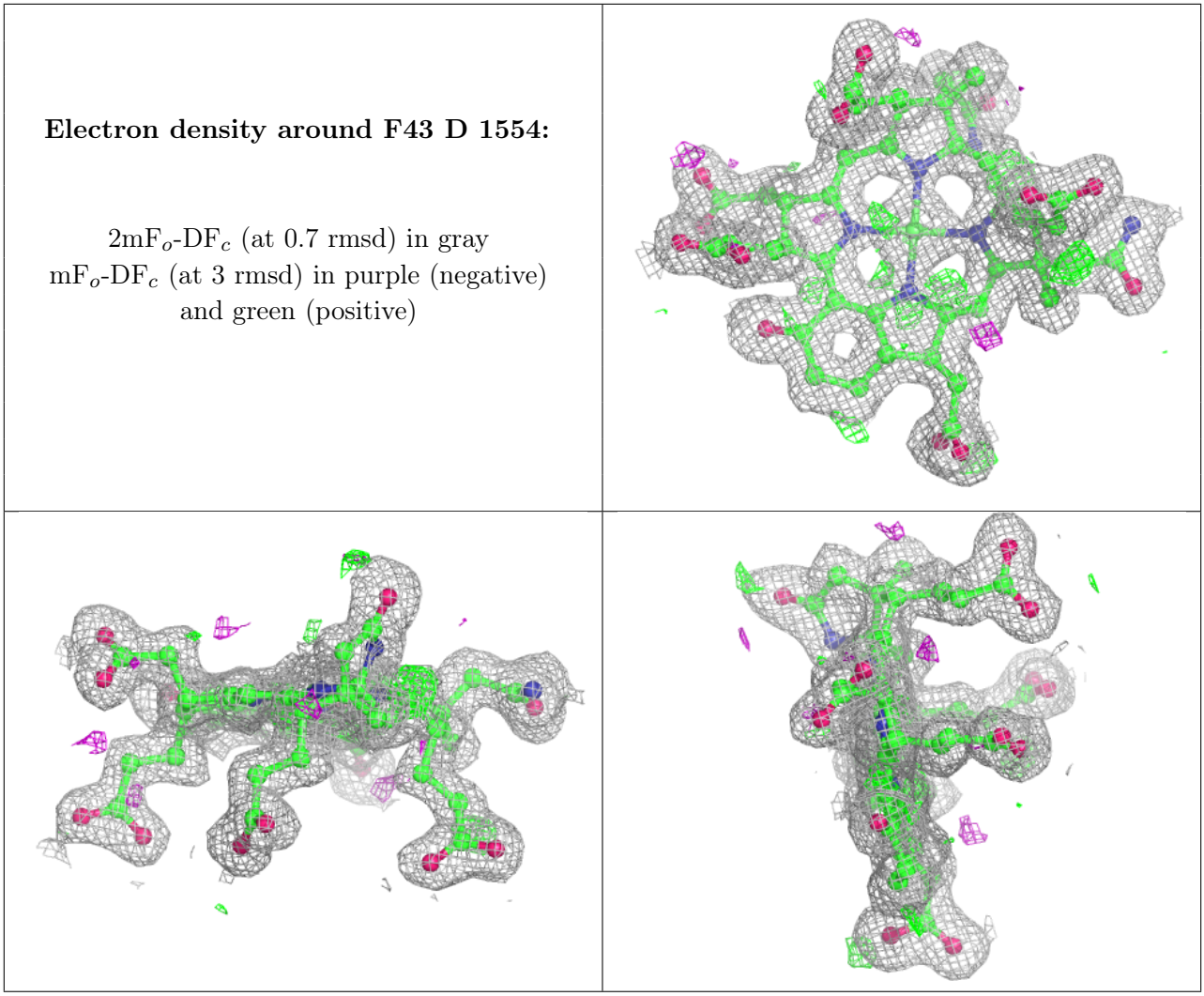






Electron density around F43 D 1554:

$2mF_o$-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.