



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2024 – 01:56 AM EDT

PDB ID : 7NKG  
Title : Methyl-coenzyme M reductase from Methermicoccus shengliensis at 1.6-Å resolution  
Authors : Mueller, M.; Wagner, T.  
Deposited on : 2021-02-18  
Resolution : 1.60 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

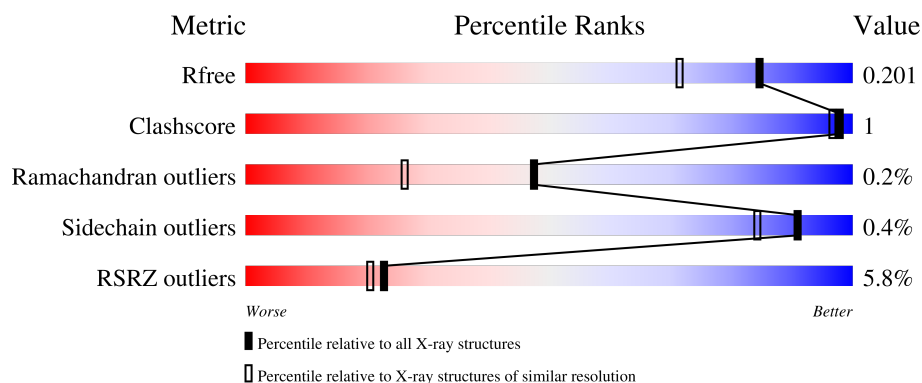
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div></div> <div>96%</div> <div>..</div> </div>
1	D	569	<div> <div></div> <div>97%</div> <div>..</div> </div>
1	G	569	<div> <div>14%</div> <div>96%</div> <div>..</div> </div>
1	J	569	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
2	B	433	<div> <div></div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	433	<div><div></div><div>99%</div><div>.</div></div>
2	H	433	<div><div>11%</div><div></div><div>99%</div><div>.</div></div>
2	K	433	<div><div>11%</div><div></div><div>98%</div><div>.</div></div>
3	C	248	<div><div>2%</div><div></div><div>98%</div><div>.</div></div>
3	F	248	<div><div>%</div><div></div><div>98%</div><div>.</div></div>
3	I	248	<div><div>9%</div><div></div><div>94%</div><div>.</div><div>.</div></div>
3	L	248	<div><div>17%</div><div></div><div>96%</div><div>.</div><div>.</div></div>

## 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:  $C_3H_8O_3$ ).

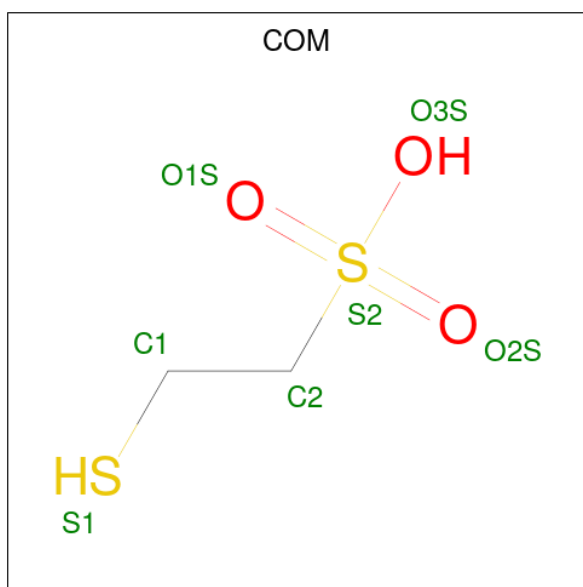


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

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

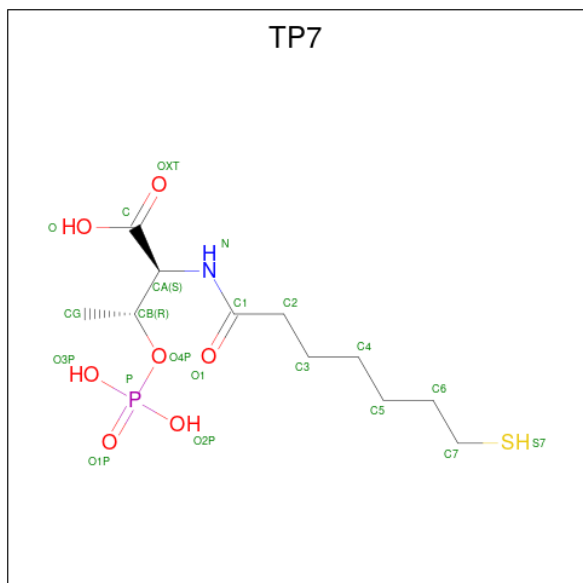
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	G	1	Total	K	0	0
			1	1		

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



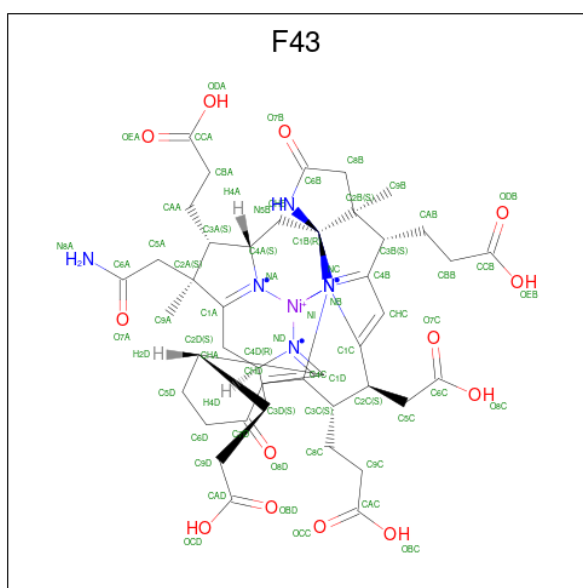
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		
6	G	1	Total	C	O	S	0	0
			7	2	3	2		
6	J	1	Total	C	O	S	0	0
			7	2	3	2		

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



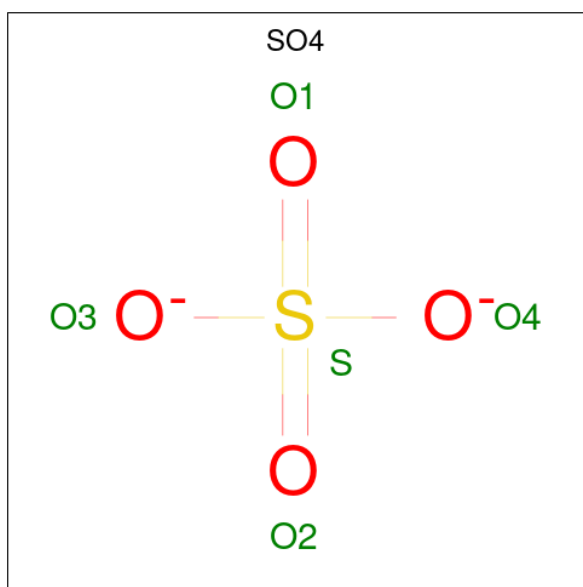
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
7	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
7	G	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
7	G	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- 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	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

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

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

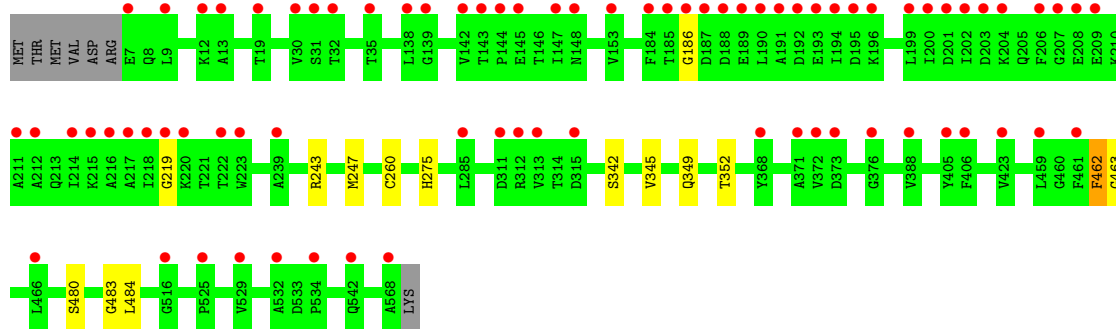
- Molecule 1: Methyl-coenzyme M reductase alpha subunit



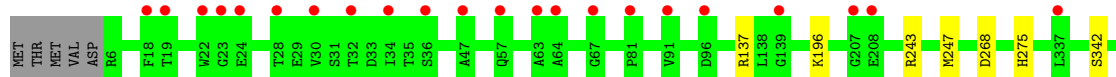
- Molecule 1: Methyl-coenzyme M reductase alpha subunit

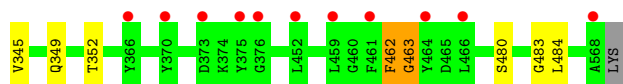


- Molecule 1: Methyl-coenzyme M reductase alpha subunit



- Molecule 1: Methyl-coenzyme M reductase alpha subunit





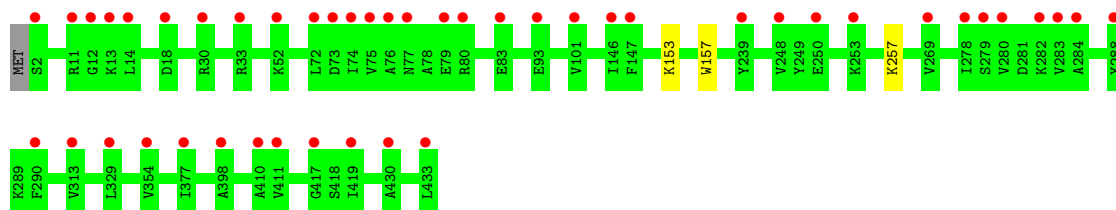
- Molecule 2: Methyl-coenzyme M reductase beta subunit



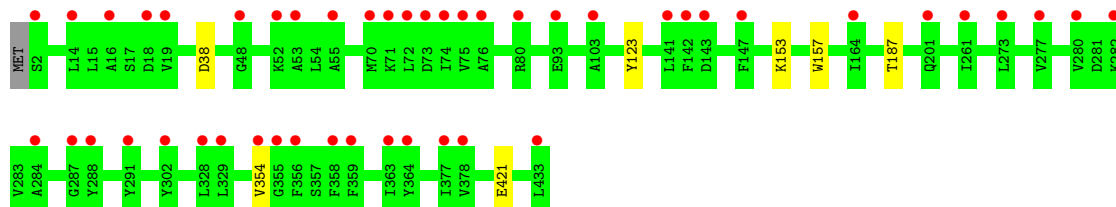
- Molecule 2: Methyl-coenzyme M reductase beta subunit



- Molecule 2: Methyl-coenzyme M reductase beta subunit



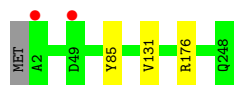
- Molecule 2: Methyl-coenzyme M reductase beta subunit



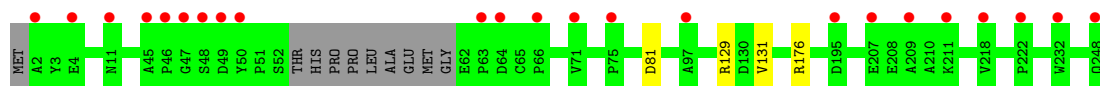
- Molecule 3: Methyl-coenzyme M reductase gamma subunit



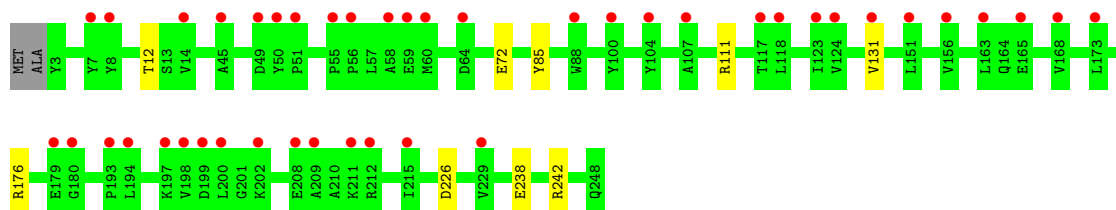
- Molecule 3: Methyl-coenzyme M reductase gamma subunit



- Molecule 3: Methyl-coenzyme M reductase gamma subunit



- Molecule 3: Methyl-coenzyme M reductase gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MHS, GOL, SO4, TP7, GL3, K, F43, AGM, 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	0.42	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

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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/440 (100%)	439 (100%)	1 (0%)	93	88
1	D	440/440 (100%)	439 (100%)	1 (0%)	93	88
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	462	PHE
2	H	257	LYS
3	L	176	ARG
1	J	462	PHE
3	L	131	VAL

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 ⓘ

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	MHS	A	275	1	7,11,12	0.58	0	6,14,16	1.32	1 (16%)
1	GL3	J	463	1	2,3,4	3.31	1 (50%)	1,2,4	0.15	0
1	AGM	A	289	1	10,11,12	0.33	0	6,13,15	0.30	0
1	MHS	J	275	1	7,11,12	0.56	0	6,14,16	1.32	1 (16%)
1	AGM	D	289	1	10,11,12	0.35	0	6,13,15	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MHS	D	275	1	7,11,12	0.68	0	6,14,16	1.33	0
1	GL3	A	463	1	2,3,4	3.31	1 (50%)	1,2,4	0.20	0
1	GL3	D	463	1	2,3,4	3.68	1 (50%)	1,2,4	0.25	0
1	MHS	G	275	1	7,11,12	0.52	0	6,14,16	1.32	1 (16%)
1	GL3	G	463	1	2,3,4	3.45	1 (50%)	1,2,4	0.28	0
1	AGM	G	289	1	10,11,12	0.32	0	6,13,15	0.31	0
1	AGM	J	289	1	10,11,12	0.34	0	6,13,15	0.25	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
1	MHS	A	275	1	-	0/5/6/8	0/1/1/1
1	GL3	J	463	1	-	1/1/1/2	-
1	AGM	A	289	1	-	0/10/11/13	-
1	MHS	J	275	1	-	0/5/6/8	0/1/1/1
1	AGM	D	289	1	-	0/10/11/13	-
1	MHS	D	275	1	-	0/5/6/8	0/1/1/1
1	GL3	A	463	1	-	0/1/1/2	-
1	GL3	D	463	1	-	1/1/1/2	-
1	MHS	G	275	1	-	0/5/6/8	0/1/1/1
1	GL3	G	463	1	-	1/1/1/2	-
1	AGM	G	289	1	-	0/10/11/13	-
1	AGM	J	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(°)	Ideal(°)
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	61,71,71	2.12	7 (11%)	64,118,118	1.44	12 (18%)
9	SO4	H	501	-	4,4,4	0.34	0	6,6,6	0.07	0
8	F43	D	602	6,1	61,71,71	2.17	6 (9%)	64,118,118	1.44	9 (14%)
9	SO4	B	501	-	4,4,4	0.35	0	6,6,6	0.14	0
9	SO4	E	501	-	4,4,4	0.35	0	6,6,6	0.16	0
8	F43	J	602	6,1	61,71,71	2.10	6 (9%)	64,118,118	1.39	11 (17%)
7	TP7	G	603	-	19,20,20	0.74	0	24,26,26	0.73	0
7	TP7	G	604	-	19,20,20	0.72	0	24,26,26	0.84	0
6	COM	J	601	8	6,6,6	1.44	2 (33%)	7,8,8	2.43	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	COM	D	601	8	6,6,6	1.41	2 (33%)	7,8,8	2.23	3 (42%)
9	SO4	E	503	-	4,4,4	0.39	0	6,6,6	0.21	0
4	GOL	A	601	-	5,5,5	0.26	0	5,5,5	0.26	0
6	COM	G	602	8	6,6,6	1.50	2 (33%)	7,8,8	2.29	2 (28%)
9	SO4	K	501	-	4,4,4	0.36	0	6,6,6	0.05	0
8	F43	A	606	6,1	61,71,71	2.21	6 (9%)	64,118,118	1.38	9 (14%)
4	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.30	0
4	GOL	E	502	-	5,5,5	0.27	0	5,5,5	0.34	0
7	TP7	A	604	-	19,20,20	0.71	0	24,26,26	0.69	0
7	TP7	A	605	-	19,20,20	0.72	0	24,26,26	0.70	0
6	COM	A	603	8	6,6,6	1.29	0	7,8,8	1.67	2 (28%)

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	-
4	GOL	E	502	-	-	0/4/4/4	-
7	TP7	A	604	-	-	1/24/24/24	-
8	F43	G	605	6,1	-	7/28/185/185	-
8	F43	J	602	6,1	-	7/28/185/185	-
7	TP7	A	605	-	-	0/24/24/24	-
7	TP7	G	603	-	-	1/24/24/24	-
7	TP7	G	604	-	-	1/24/24/24	-
8	F43	D	602	6,1	-	5/28/185/185	-
6	COM	A	603	8	-	0/4/4/4	-
4	GOL	A	601	-	-	2/4/4/4	-
6	COM	G	602	8	-	0/4/4/4	-
6	COM	J	601	8	-	0/4/4/4	-
8	F43	A	606	6,1	-	7/28/185/185	-
6	COM	D	601	8	-	0/4/4/4	-

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	606	F43	NI-NB	8.30	2.07	1.89
8	D	602	F43	NI-NB	8.27	2.07	1.89

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
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

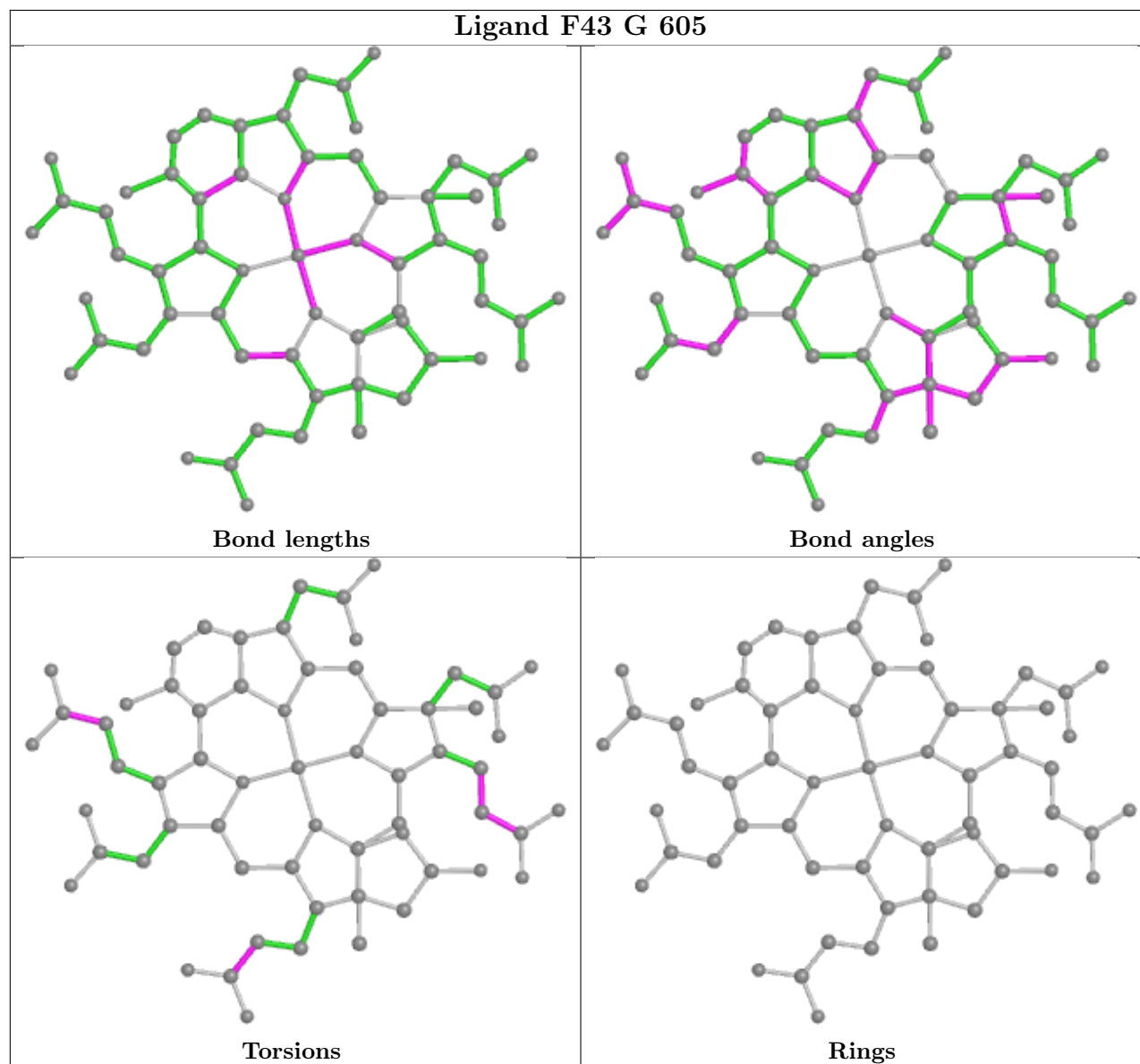
There are no ring outliers.

9 monomers are involved in 15 short contacts:

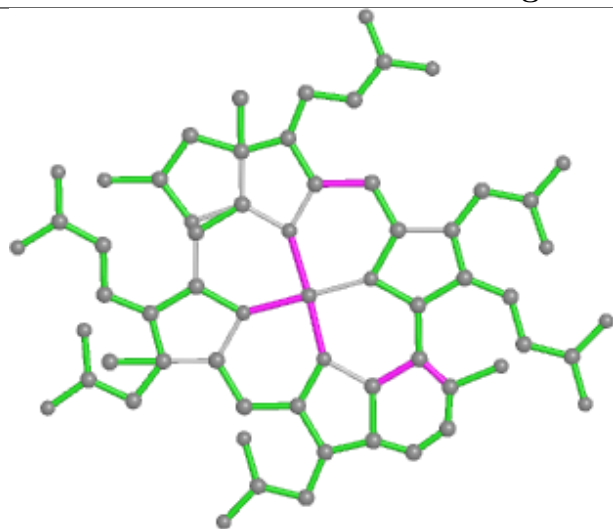
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	605	F43	4	0
8	D	602	F43	1	0
9	E	501	SO4	1	0
8	J	602	F43	3	0
6	J	601	COM	3	0
6	D	601	COM	2	0
6	G	602	COM	3	0
8	A	606	F43	2	0
7	A	604	TP7	1	0

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

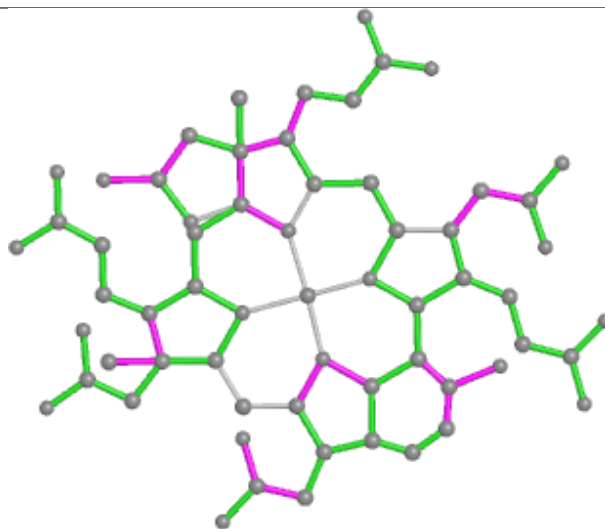
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



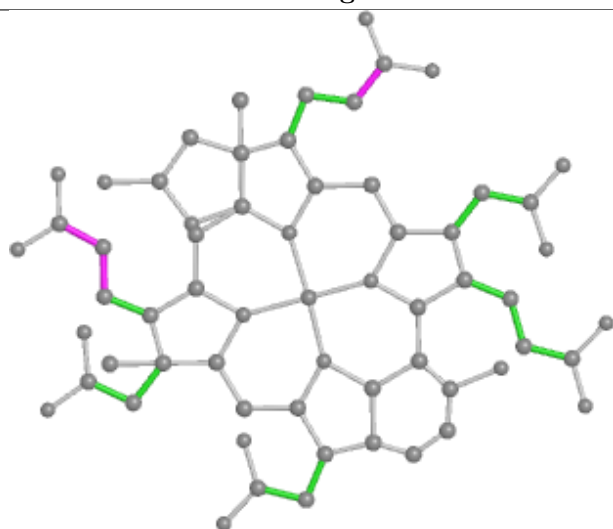
## Ligand F43 D 602



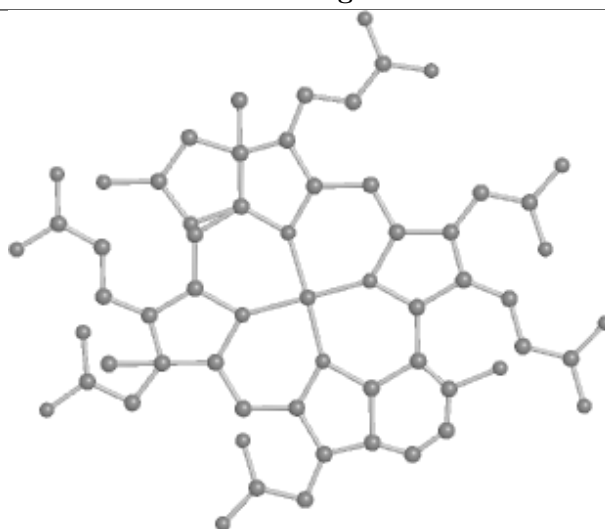
Bond lengths



Bond angles

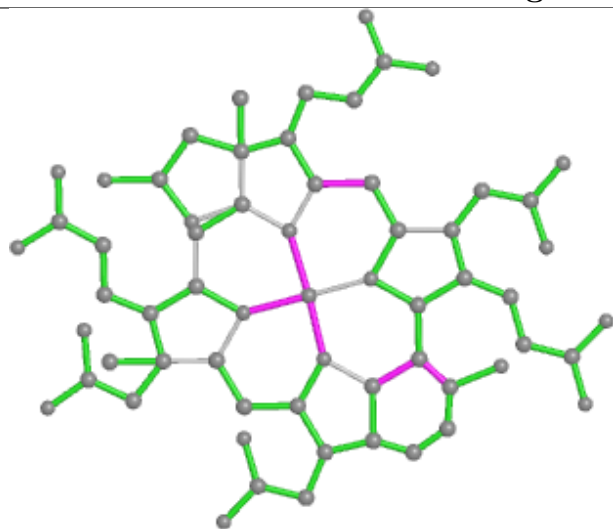


Torsions

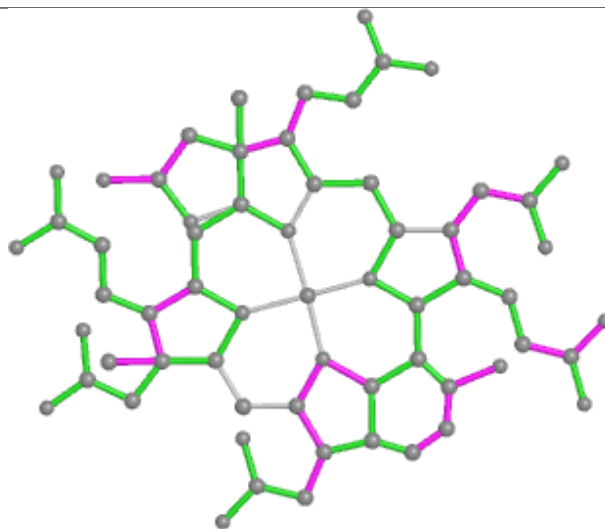


Rings

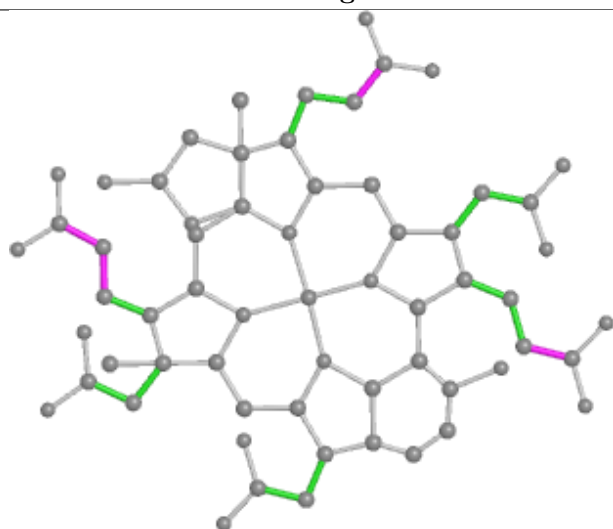
## Ligand F43 J 602



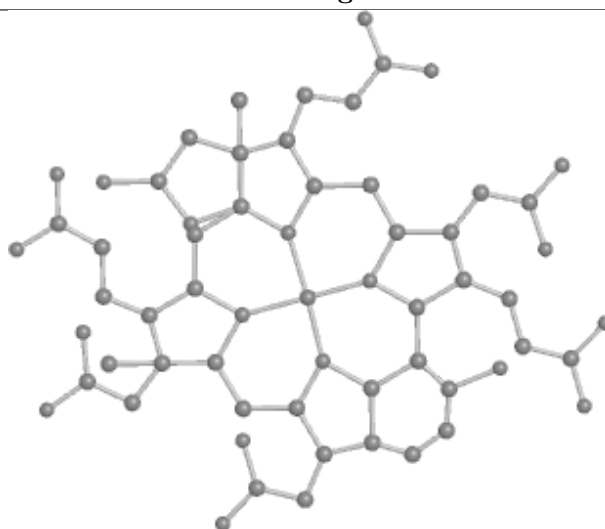
Bond lengths



Bond angles

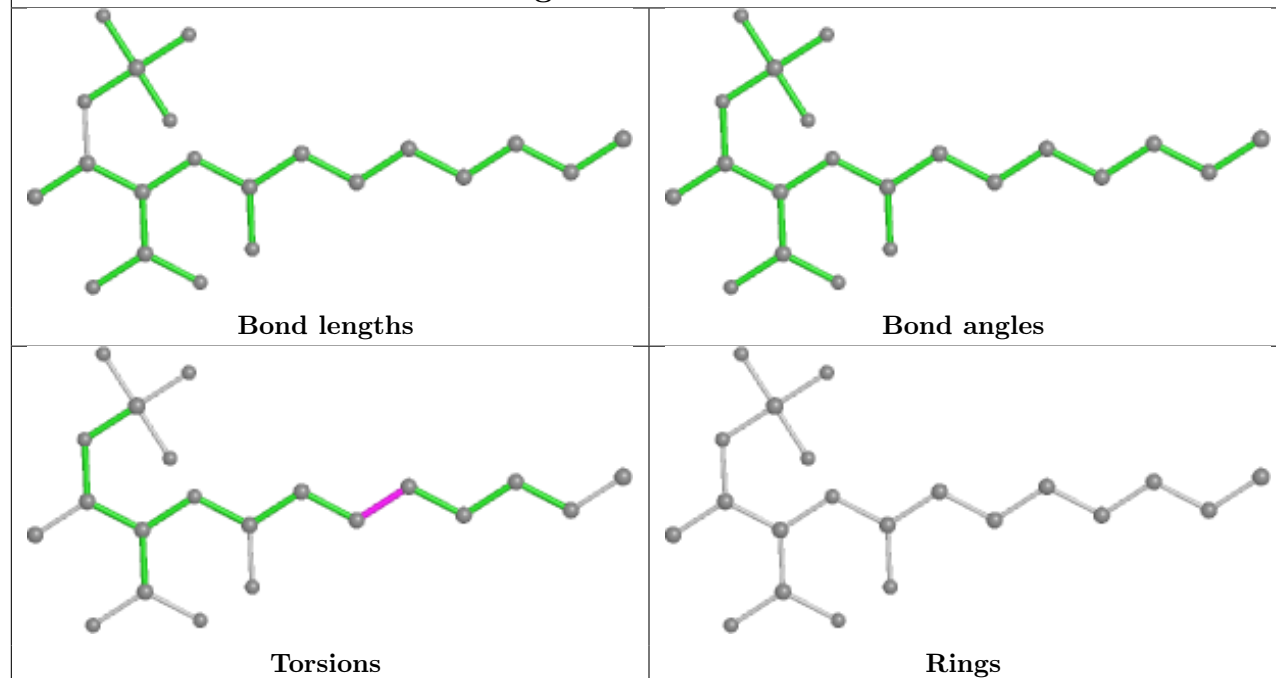


Torsions

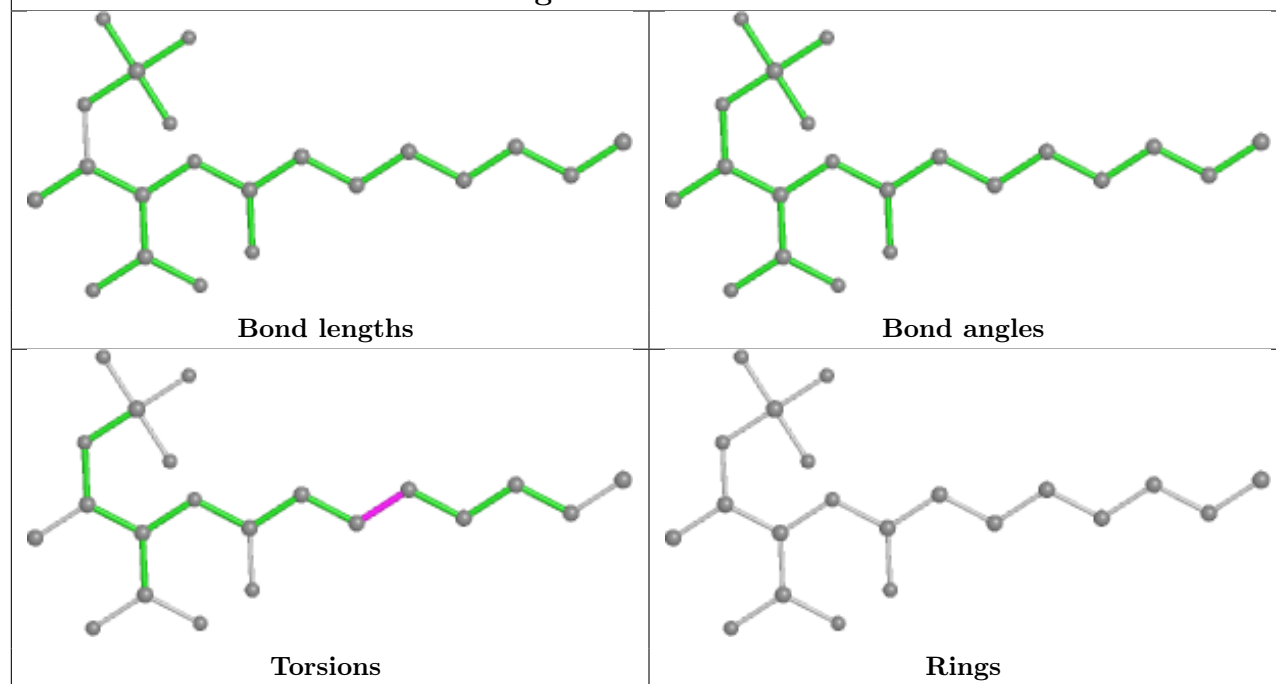


Rings

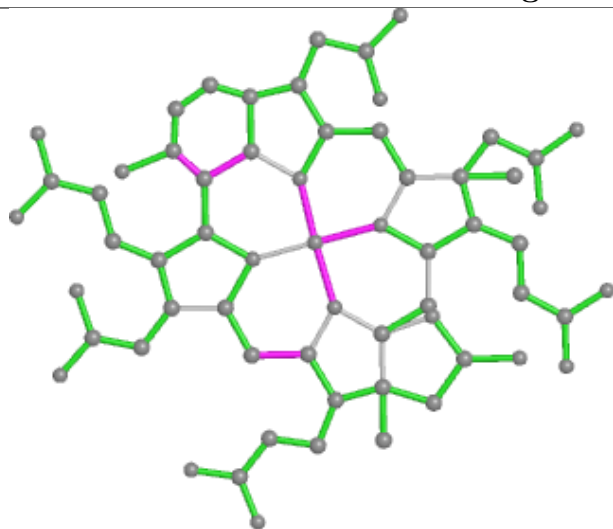
## Ligand TP7 G 603



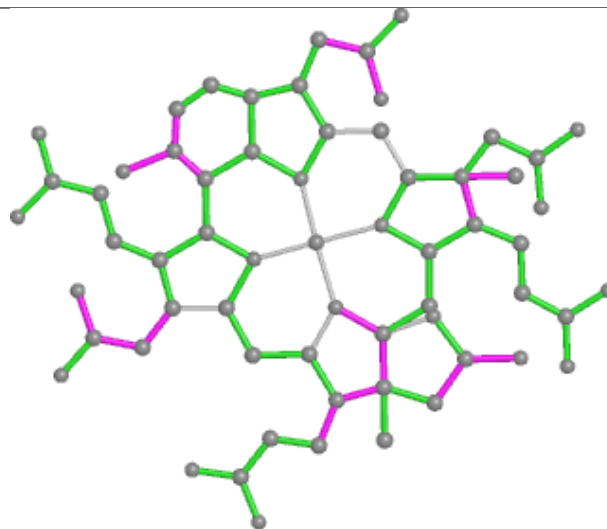
## Ligand TP7 G 604



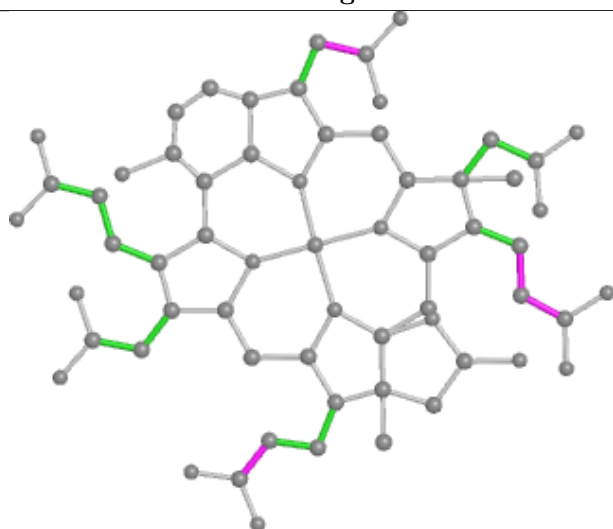
## Ligand F43 A 606



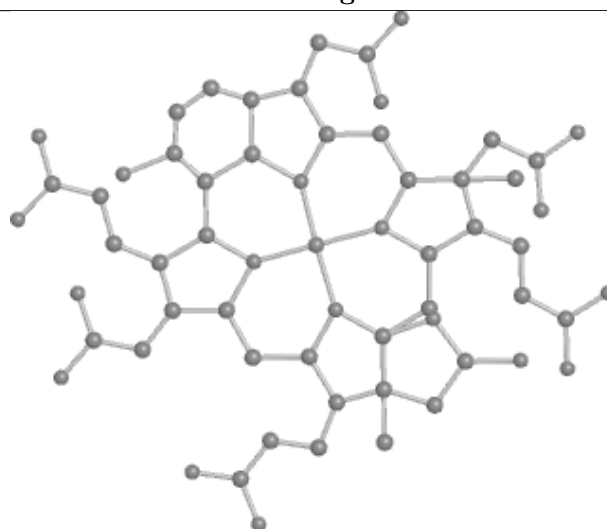
Bond lengths



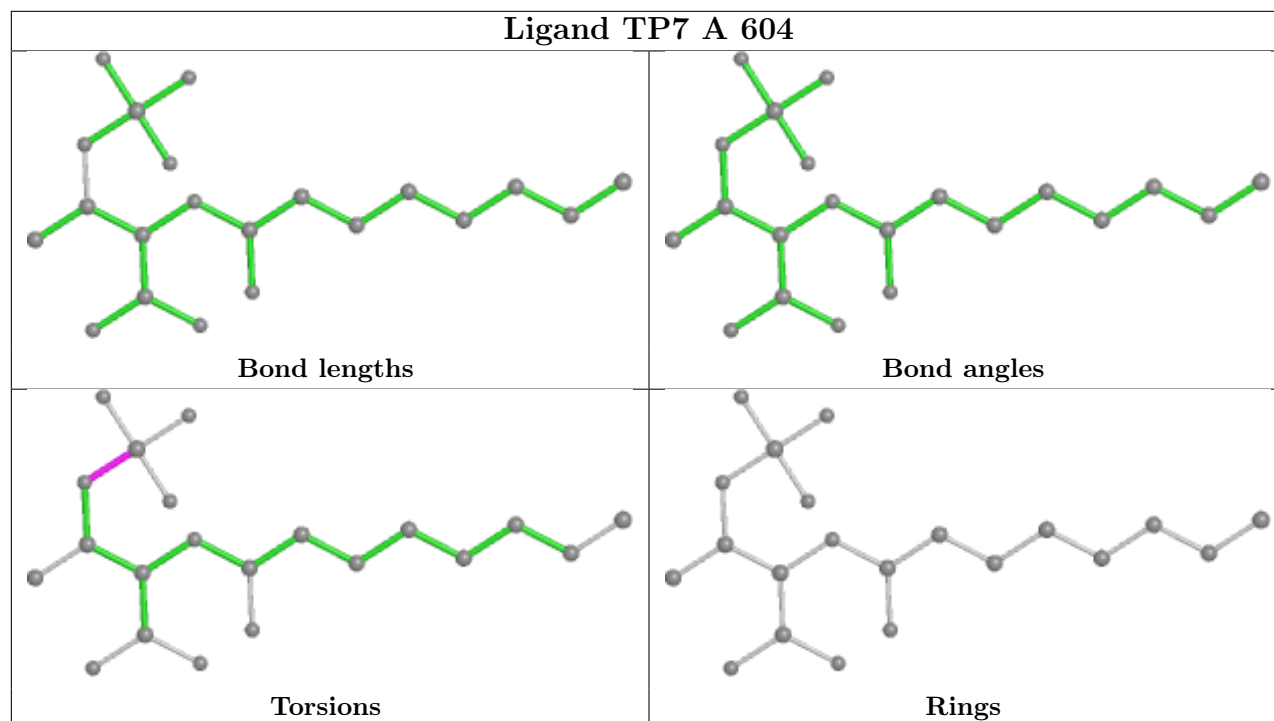
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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

The worst 5 of 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

### 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<sup>th</sup> 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 <sup>2</sup> )	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
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<sup>th</sup> 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 <sup>2</sup> )	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

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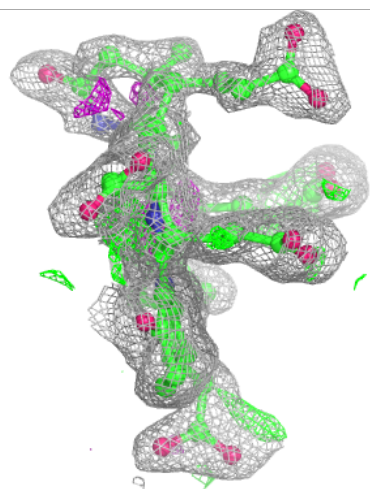
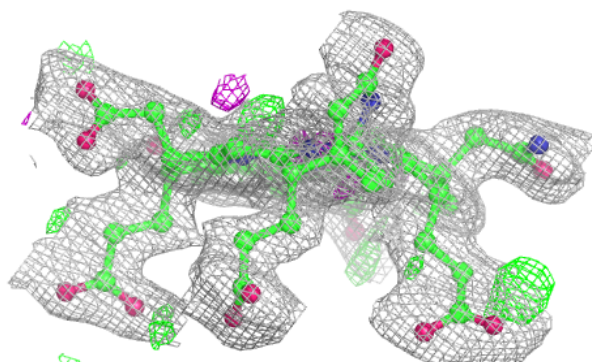
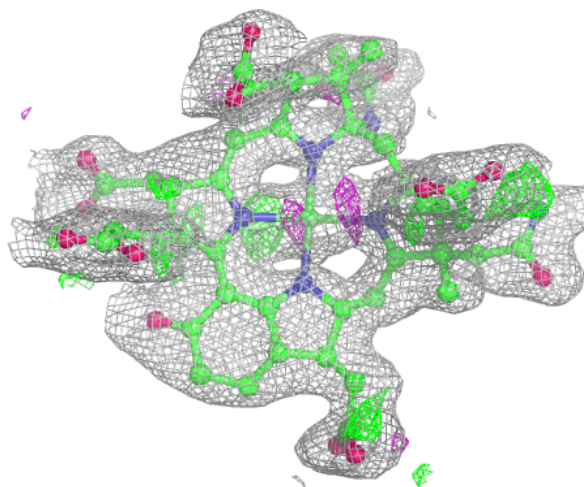
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	COM	A	603	7/7	0.97	0.09	20,21,21,22	0
8	F43	A	606	62/62	0.97	0.10	14,16,19,21	0
7	TP7	A	604	21/21	0.97	0.11	16,17,18,19	0
7	TP7	A	605	21/21	0.97	0.10	15,17,18,18	0
8	F43	D	602	62/62	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.

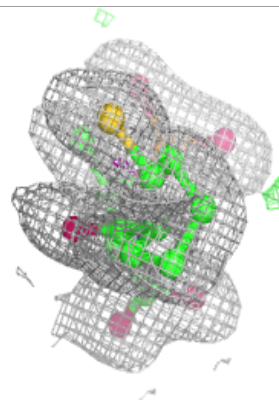
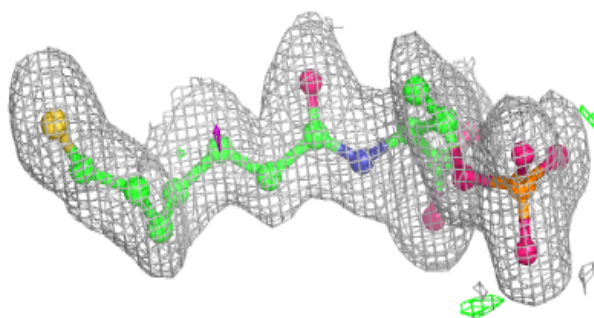
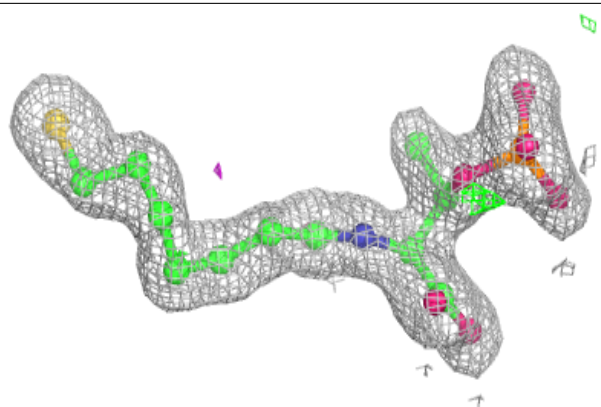
**Electron density around F43 G 605:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



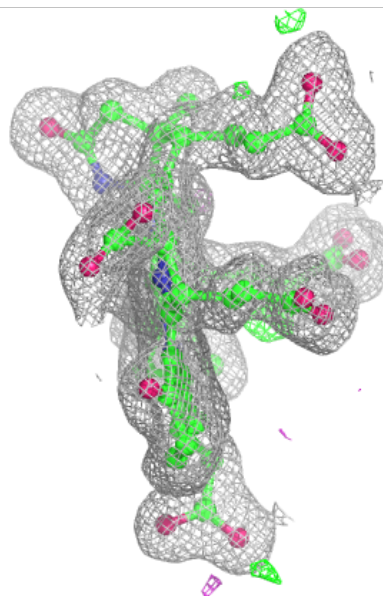
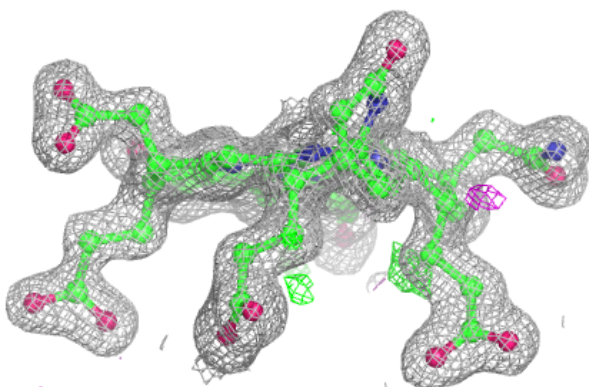
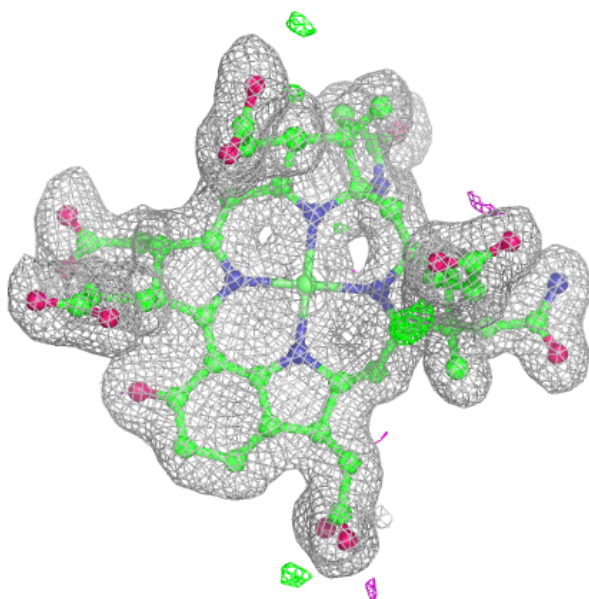
**Electron density around TP7 G 604:**

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



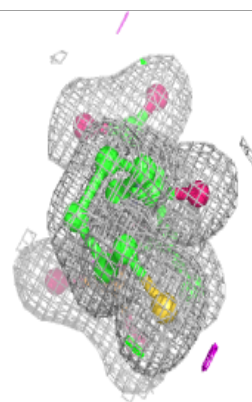
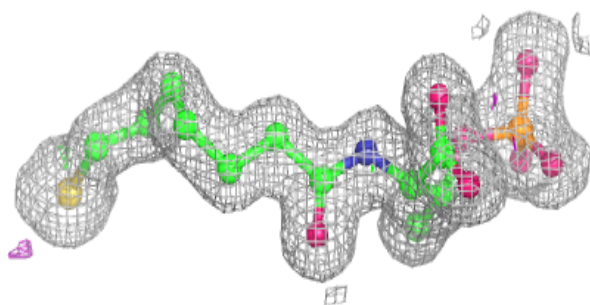
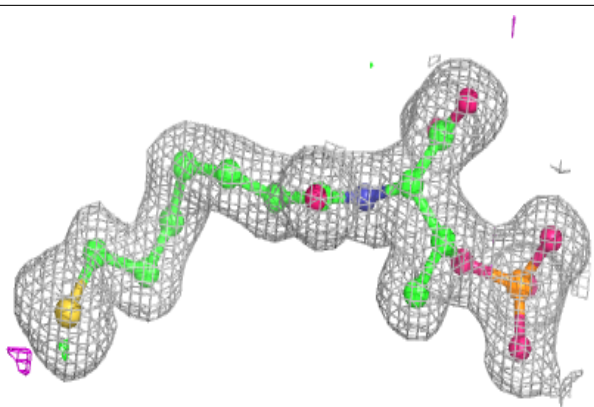
**Electron density around F43 J 602:**

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



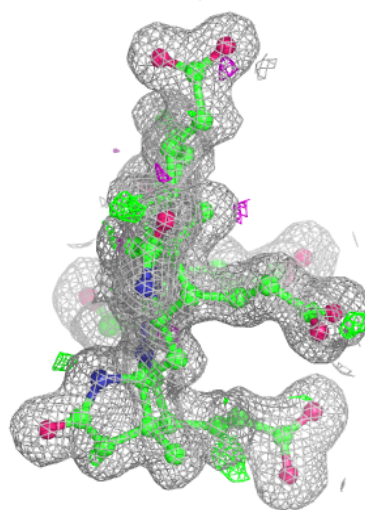
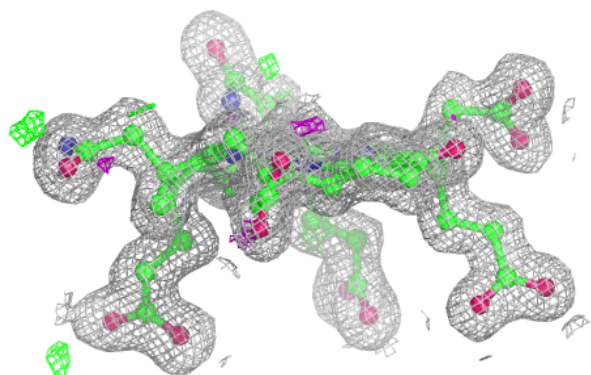
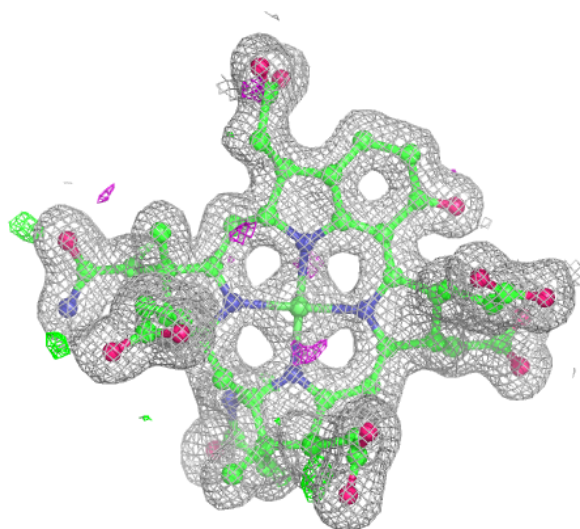
**Electron density around TP7 G 603:**

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



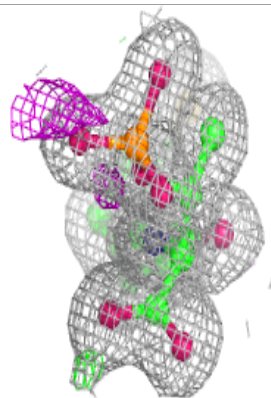
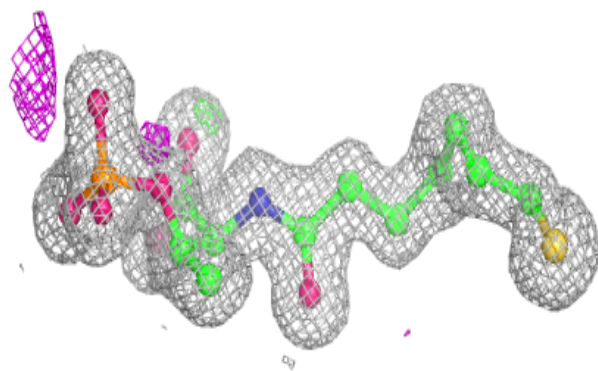
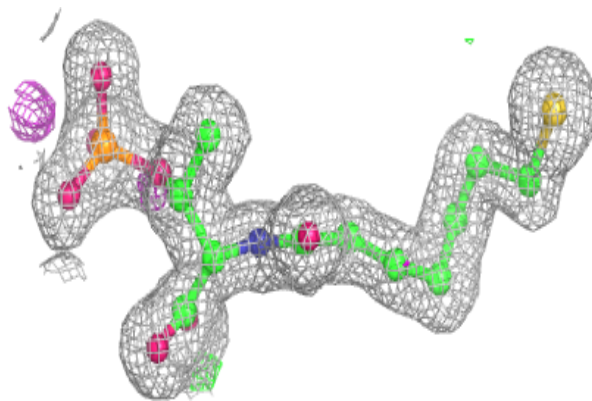
**Electron density around F43 A 606:**

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



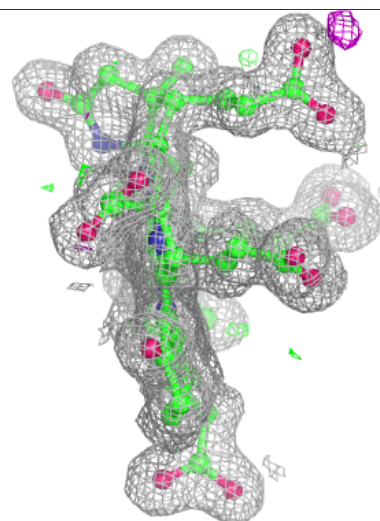
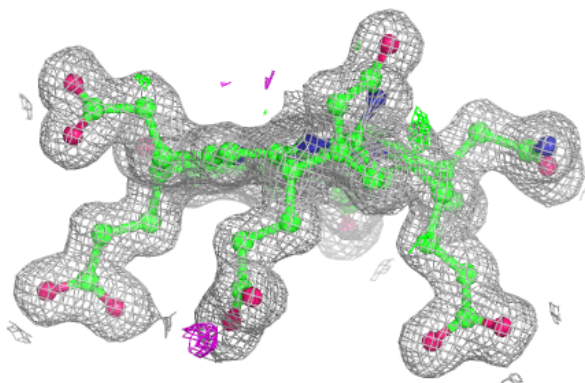
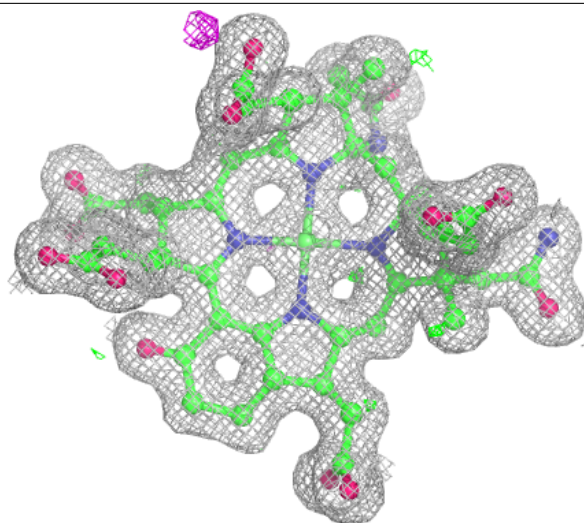
**Electron density around TP7 A 604:**

$2mF_o-DF_c$  (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 [i](#)

There are no such residues in this entry.