wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2026 – 06:26 PM EDT

PDB ID	:	9OQC / pdb_00009oqc
Title	:	Methyl-coenzyme M Reductase red1/red1-silent ensemble cryo-capillary
Authors	:	Ohmer, C.J.; Ragsdale, S.W.
Deposited on	:	2025-05-20
Resolution	:	1.55 Å(reported)

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

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

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

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

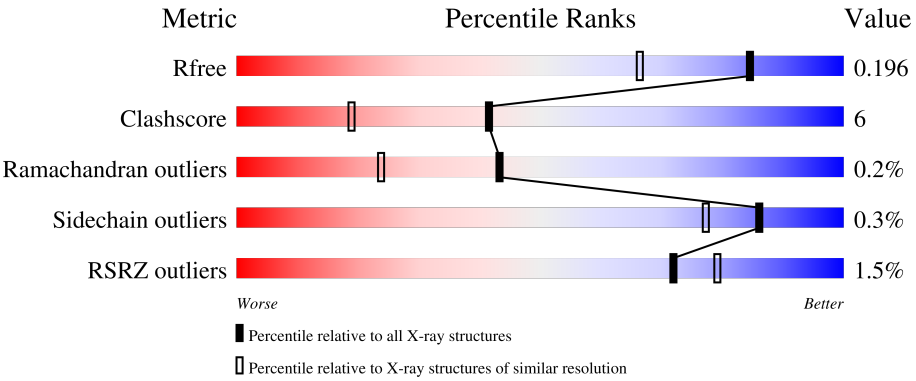
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	548	72% 27%
1	a	548	78% 22%
2	B	442	77% 23%
2	b	442	3% 70% 29%
3	C	248	2% 77% 23%

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Mol	Chain	Length	Quality of chain
3	c	248	3% 75% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	DYA	A	450[A]	-	X	-	-
1	DYA	A	450[W]	-	X	-	-
1	DYA	a	450[A]	-	X	-	-
1	DYA	a	450[W]	-	X	-	-
5	COM	a	604[A]	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 77998 atoms, of which 37346 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 I subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	548	Total	C	H	N	O	S	0	548	0
			16619	5382	8117	1428	1652	40			
1	a	548	Total	C	H	N	O	S	0	548	0
			16620	5382	8118	1428	1652	40			

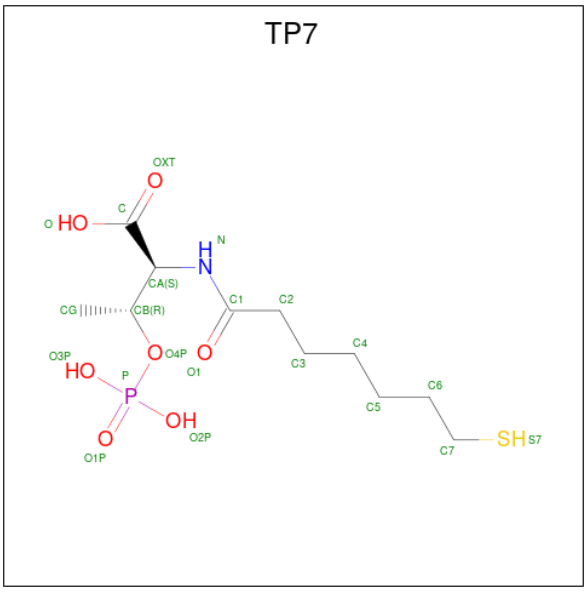
- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	442	Total	C	H	N	O	S	0	442	0
			13204	4184	6590	1098	1296	36			
2	b	442	Total	C	H	N	O	S	0	442	0
			13197	4184	6583	1098	1296	36			

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

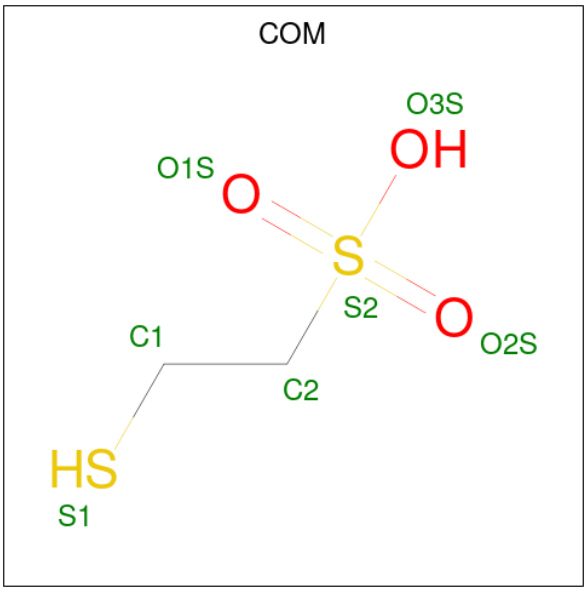
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	248	0
			7885	2486	3869	710	798	22			
3	c	248	Total	C	H	N	O	S	0	248	0
			7883	2486	3867	710	798	22			

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	S	0	1
			40	11	19	1	7	1	1		
4	a	1	Total	C	H	N	O	P	S	0	0
			40	11	19	1	7	1	1		

- Molecule 5 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



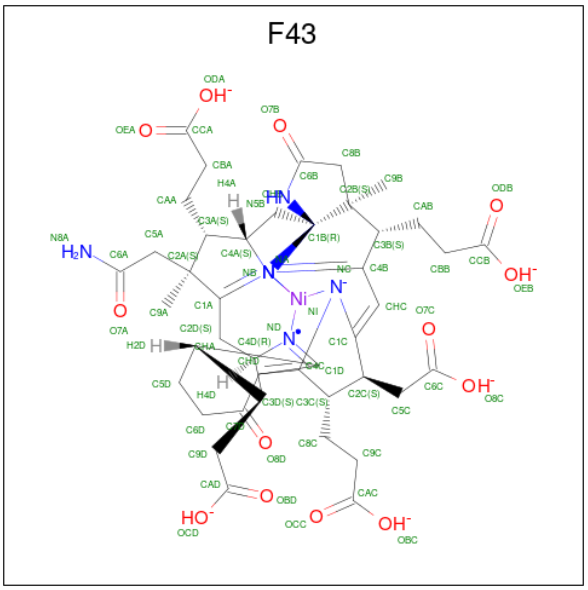
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	1
			22	4	8	6	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	a	1	Total	C	H	O	S	0	1
			20	4	6	6	4		

- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	Ni	O	0	1
			89	42	27	6	1	13		
6	a	1	Total	C	H	N	Ni	O	0	1
			219	84	95	12	2	26		
6	a	1	Total	C	H	N	Ni	O	0	1
			90	42	28	6	1	13		

- Molecule 7 is TITANIUM ION (CCD ID: 4TI) (formula: Ti).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ti	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	C	1	Total Mg 1 1	0	0
8	a	1	Total Mg 1 1	0	0
8	b	1	Total Mg 1 1	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0
9	C	1	Total Na 1 1	0	0
9	a	2	Total Na 2 2	0	0

- Molecule 10 is water.

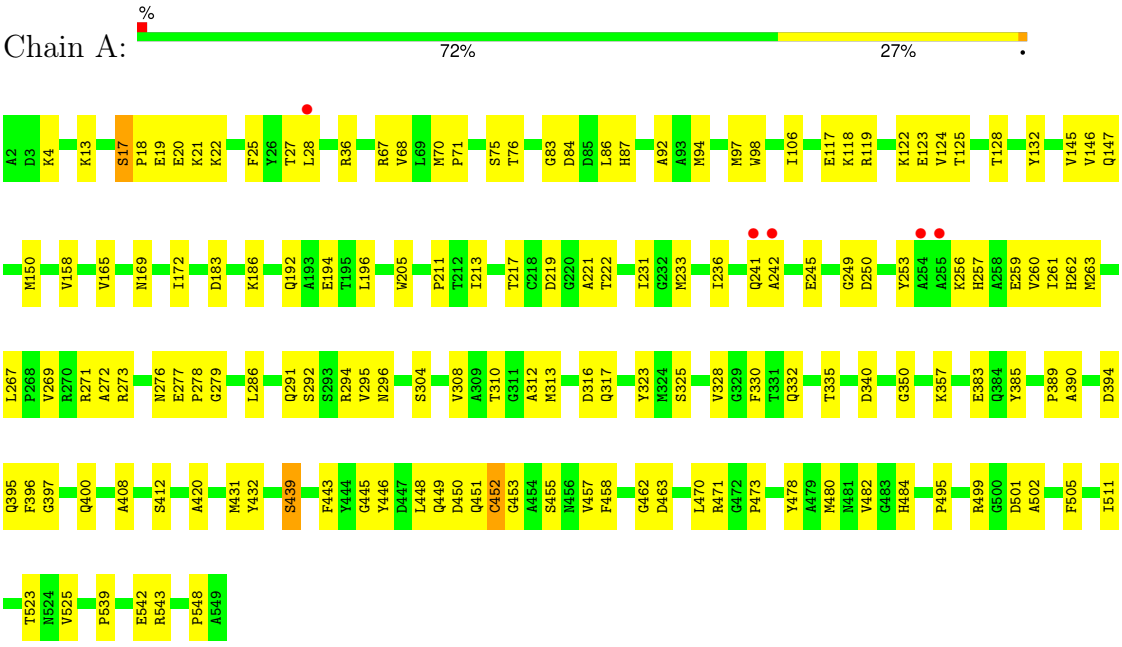
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	479	Total O 494 494	0	54
10	B	333	Total O 349 349	0	53
10	C	196	Total O 205 205	0	33
10	a	511	Total O 530 530	0	68
10	b	304	Total O 325 325	0	69
10	c	146	Total O 153 153	0	37

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.

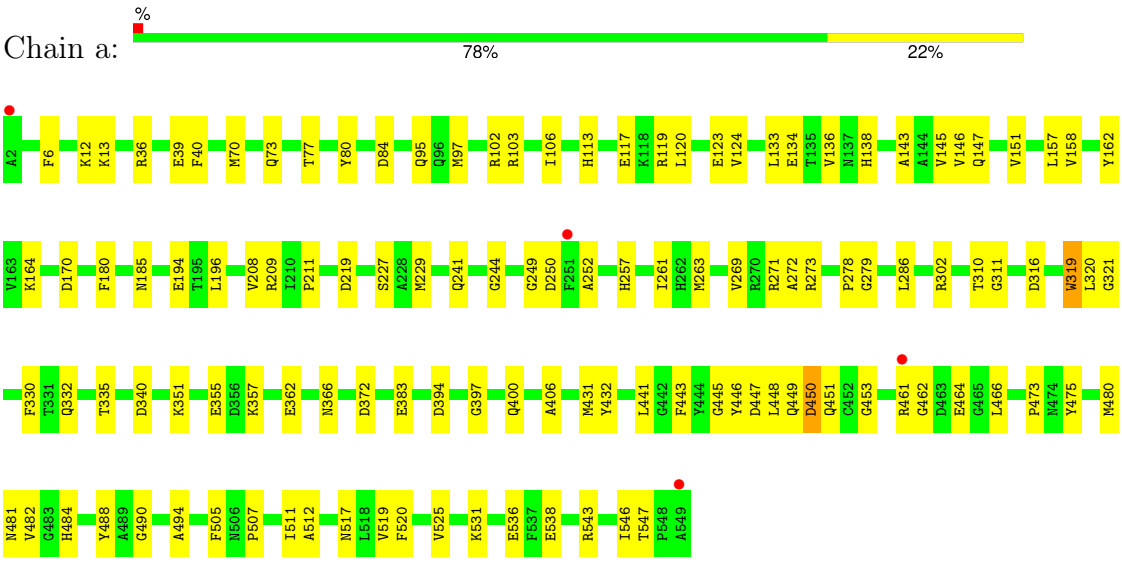
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain A:



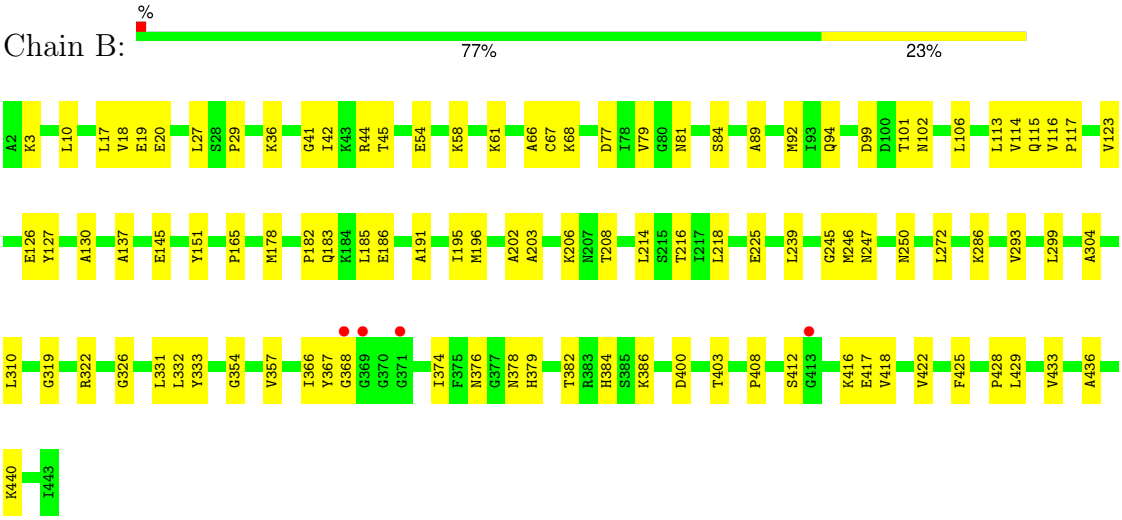
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain a:



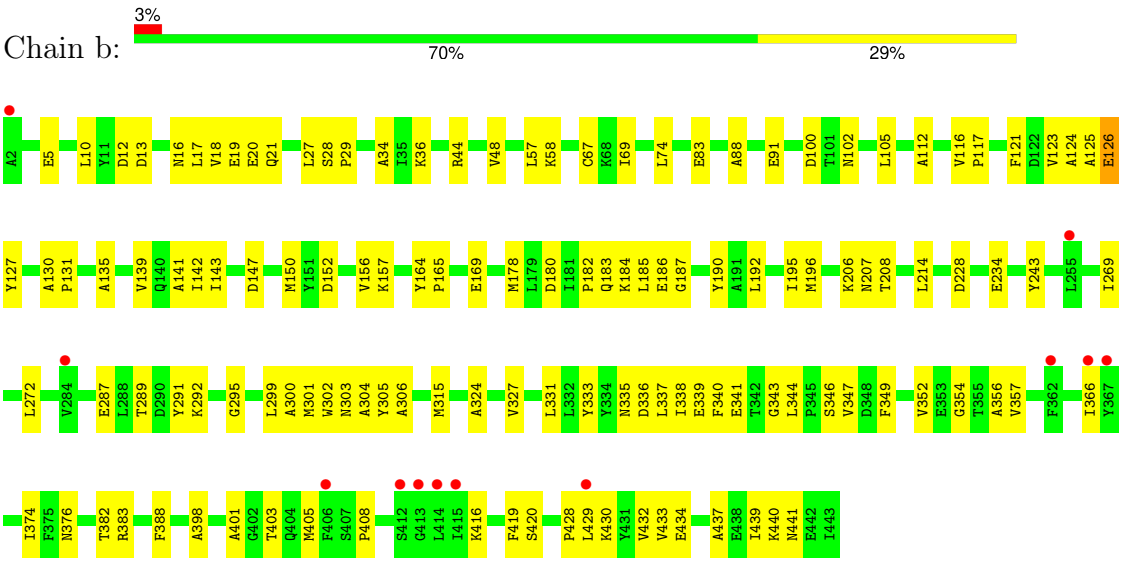
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain B:



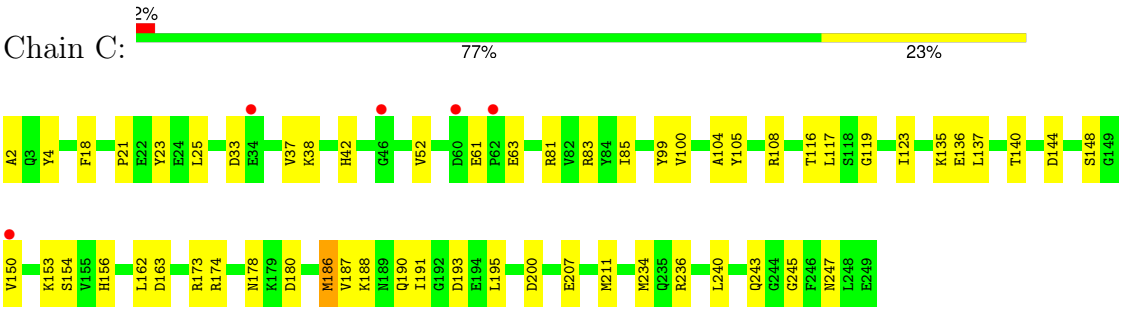
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain b:



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

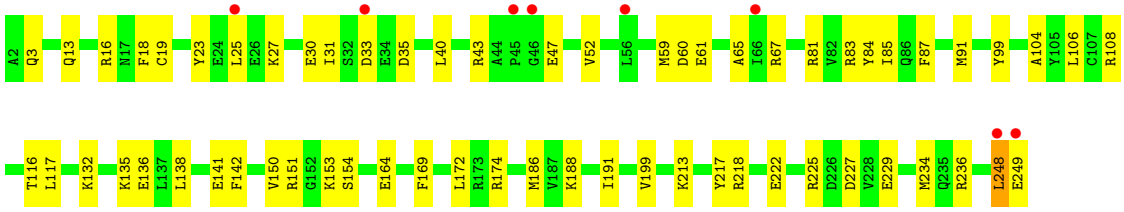
Chain C:



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

Chain c:




A2 Q3 Q13 R16 N17 F18 C19 Y23 E24 L25 E26 K27 E30 I31 S32 D33 E34 D35 L40 R43 A44 P45 G46 E47 V52 L56 M59 D60 E61 A65 I66 R67 R81 V82 R83 Y84 I85 Q86 F87 M91 Y99 A104 Y105 L106 C107 R108
T116 L117 K132 K135 E136 L137 L138 E141 F142 V150 R151 G152 K153 S154 E164 F169 L172 R173 R174 M186 V187 K188 I191 V199 K213 Y217 R218 E222 R225 D226 D227 V228 E229 M234 Q235 R236 L248 E249

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.78Å 117.49Å 123.99Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	41.29 – 1.55 41.29 – 1.55	Depositor EDS
% Data completeness (in resolution range)	94.0 (41.29-1.55) 94.0 (41.29-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.154 , 0.196 0.155 , 0.196	Depositor DCC
R_{free} test set	16988 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	77998	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MGN, AGM, GL3, TP7, MHS, SMC, 4TI, F43, DYA, NA, 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	0.15	0/8586	0.34	0/11652
1	a	0.15	0/8586	0.35	0/11652
2	B	0.13	0/6716	0.31	0/9100
2	b	0.13	0/6716	0.29	0/9100
3	C	0.13	0/4088	0.32	0/5508
3	c	0.11	0/4088	0.29	0/5508
All	All	0.14	0/38780	0.32	0/52520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8502	8117	8112	120	0
1	a	8502	8118	8113	108	0
2	B	6614	6590	6589	91	0
2	b	6614	6583	6583	124	0
3	C	4016	3869	3869	50	0
3	c	4016	3867	3867	55	0
4	A	21	19	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	a	21	19	19	4	0
5	A	14	8	10	1	0
5	a	14	6	11	1	0
6	A	62	27	23	9	0
6	a	186	123	112	5	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	a	1	0	0	0	0
8	b	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	a	2	0	0	0	0
10	A	494	0	0	11	1
10	B	349	0	0	21	2
10	C	205	0	0	13	0
10	a	530	0	0	16	1
10	b	325	0	0	21	0
10	c	153	0	0	9	0
All	All	40652	37346	37327	485	2

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 6.

The worst 5 of 485 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)
1:A:233[W]:MET:HE3	2:b:366[W]:ILE:HD13	1.38	1.02
2:B:115[W]:GLN:NE2	10:B:866[W]:HOH:O	1.97	0.97
2:B:126[W]:GLU:OE1	10:B:601:HOH:O	1.81	0.97
1:A:233[W]:MET:HE2	2:b:366[W]:ILE:HG21	1.48	0.95
3:C:193[W]:ASP:OD2	10:C:401:HOH:O	1.86	0.94

All (2) 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)
10:B:737:HOH:O	10:a:957:HOH:O[1_655]	2.12	0.08
10:A:1030:HOH:O	10:B:895:HOH:O[1_455]	2.13	0.07

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	1080/548 (197%)	1018 (94%)	62 (6%)	0	100 100
1	a	1080/548 (197%)	1020 (94%)	54 (5%)	6 (1%)	21 6
2	B	880/442 (199%)	846 (96%)	34 (4%)	0	100 100
2	b	880/442 (199%)	842 (96%)	34 (4%)	4 (0%)	24 8
3	C	492/248 (198%)	466 (95%)	26 (5%)	0	100 100
3	c	492/248 (198%)	466 (95%)	24 (5%)	2 (0%)	30 13
All	All	4904/2476 (198%)	4658 (95%)	234 (5%)	12 (0%)	43 24

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17[A]	LEU
2	b	17[W]	LEU
1	a	319[A]	TRP
1	a	319[W]	TRP
3	c	248[A]	LEU

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	864/432 (200%)	860 (100%)	4 (0%)	81 68
1	a	864/432 (200%)	862 (100%)	2 (0%)	87 79
2	B	682/341 (200%)	682 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	682/341 (200%)	680 (100%)	2 (0%)	86	77
3	C	432/216 (200%)	430 (100%)	2 (0%)	81	68
3	c	432/216 (200%)	430 (100%)	2 (0%)	81	68
All	All	3956/1978 (200%)	3944 (100%)	12 (0%)	86	77

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	77[W]	THR
2	b	126[A]	GLU
3	c	186[W]	MET
2	b	126[W]	GLU
1	A	439[W]	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	GL3	a	445[A]	1	2,3,4	1.37	0	1,2,4	0.21	0
1	DYA	a	450[W]	1	6,7,8	2.54	2 (33%)	6,8,10	3.54	4 (66%)
1	MGN	a	400[A]	1	6,9,10	0.85	0	7,12,14	0.85	0
1	AGM	a	271[A]	1	10,11,12	1.34	1 (10%)	7,13,15	1.04	0
1	MHS	a	257[W]	1	10,11,12	1.77	1 (10%)	5,14,16	0.98	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	DYA	a	450[A]	1	6,7,8	2.58	2 (33%)	6,8,10	4.05	4 (66%)
1	MGN	A	400[W]	1	6,9,10	0.83	0	7,12,14	0.81	0
1	SMC	a	452[W]	1	5,6,7	1.02	0	3,6,8	1.43	0
1	MHS	a	257[A]	1	10,11,12	1.72	1 (10%)	5,14,16	1.41	1 (20%)
1	AGM	A	271[W]	1	10,11,12	1.34	1 (10%)	7,13,15	1.34	1 (14%)
1	GL3	A	445[W]	1	2,3,4	1.41	0	1,2,4	0.35	0
1	DYA	A	450[W]	1	6,7,8	3.11	4 (66%)	6,8,10	3.66	3 (50%)
1	MGN	A	400[A]	1	6,9,10	0.89	0	7,12,14	0.94	1 (14%)
1	SMC	a	452[A]	1	5,6,7	1.01	0	3,6,8	1.31	0
1	MHS	A	257[W]	1	10,11,12	1.79	1 (10%)	5,14,16	1.25	1 (20%)
1	SMC	A	452[W]	1	5,6,7	1.01	0	3,6,8	1.05	0
1	AGM	A	271[A]	1	10,11,12	1.31	1 (10%)	7,13,15	1.11	0
1	GL3	A	445[A]	1	2,3,4	1.45	1 (50%)	1,2,4	0.21	0
1	GL3	a	445[W]	1	2,3,4	1.29	0	1,2,4	0.58	0
1	DYA	A	450[A]	1	6,7,8	3.17	4 (66%)	6,8,10	3.83	3 (50%)
1	MHS	A	257[A]	1	10,11,12	1.84	2 (20%)	5,14,16	0.97	1 (20%)
1	MGN	a	400[W]	1	6,9,10	0.88	0	7,12,14	0.89	0
1	SMC	A	452[A]	1	5,6,7	1.05	0	3,6,8	2.03	1 (33%)
1	AGM	a	271[W]	1	10,11,12	1.33	1 (10%)	7,13,15	1.28	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GL3	a	445[A]	1	-	0/1/1/2	-
1	DYA	a	450[W]	1	-	4/4/6/8	-
1	MGN	a	400[A]	1	-	0/7/9/12	-
1	AGM	a	271[A]	1	-	2/10/11/13	-
1	MHS	a	257[W]	1	-	0/5/6/8	0/1/1/1
1	DYA	a	450[A]	1	-	4/4/6/8	-
1	MGN	A	400[W]	1	-	0/7/9/12	-
1	SMC	a	452[W]	1	-	1/3/5/7	-
1	MHS	a	257[A]	1	-	0/5/6/8	0/1/1/1
1	AGM	A	271[W]	1	-	2/10/11/13	-
1	GL3	A	445[W]	1	-	1/1/1/2	-
1	DYA	A	450[W]	1	-	4/4/6/8	-
1	MGN	A	400[A]	1	-	2/7/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	a	452[A]	1	-	1/3/5/7	-
1	MHS	A	257[W]	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452[W]	1	-	1/3/5/7	-
1	AGM	A	271[A]	1	-	3/10/11/13	-
1	GL3	A	445[A]	1	-	0/1/1/2	-
1	GL3	a	445[W]	1	-	1/1/1/2	-
1	DYA	A	450[A]	1	-	4/4/6/8	-
1	MHS	A	257[A]	1	-	0/5/6/8	0/1/1/1
1	MGN	a	400[W]	1	-	0/7/9/12	-
1	SMC	A	452[A]	1	-	1/3/5/7	-
1	AGM	a	271[W]	1	-	2/10/11/13	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450[A]	DYA	CB-CA	5.62	1.52	1.36
1	a	450[W]	DYA	CB-CA	5.55	1.52	1.36
1	A	450[W]	DYA	CB-CA	5.55	1.52	1.36
1	a	450[A]	DYA	CB-CA	5.49	1.52	1.36
1	A	257[A]	MHS	CD2-CG	3.81	1.41	1.36

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450[W]	DYA	CB-CA-N	-7.17	110.22	123.25
1	A	450[A]	DYA	O-C-CA	-6.53	117.20	125.39
1	a	450[A]	DYA	O-C-CA	-6.40	117.36	125.39
1	a	450[A]	DYA	CB-CA-N	-6.34	111.74	123.25
1	A	450[A]	DYA	CB-CA-N	-5.92	112.49	123.25

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	271[A]	AGM	CE2-CD-CG-CB
1	A	271[A]	AGM	NE1-CD-CG-CB
1	A	450[A]	DYA	N-CA-CB-CG
1	A	450[A]	DYA	O-C-CA-CB
1	A	450[W]	DYA	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	445[A]	GL3	1	0
1	a	400[A]	MGN	1	0
1	a	450[A]	DYA	2	0
1	a	445[W]	GL3	1	0
1	A	452[A]	SMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	TP7	a	602	-	19,20,20	1.51	2 (10%)	24,26,26	1.51	3 (12%)
5	COM	a	604[W]	6	6,6,6	1.50	0	8,8,8	1.55	2 (25%)
6	F43	a	601[A]	10	63,71,71	1.83	8 (12%)	73,118,118	1.55	15 (20%)
6	F43	a	601[W]	1,5	63,71,71	1.85	8 (12%)	73,118,118	1.68	16 (21%)
5	COM	A	602[A]	-	6,6,6	1.77	2 (33%)	8,8,8	1.64	2 (25%)
6	F43	a	603[W]	1,5	63,71,71	1.86	9 (14%)	73,118,118	1.79	16 (21%)
5	COM	A	602[W]	6	6,6,6	1.44	1 (16%)	8,8,8	0.91	0
4	TP7	A	601[W]	-	19,20,20	1.36	2 (10%)	24,26,26	1.27	3 (12%)
6	F43	A	603[A]	10	63,71,71	1.82	7 (11%)	73,118,118	1.68	15 (20%)
5	COM	a	604[A]	-	6,6,6	1.69	2 (33%)	8,8,8	1.41	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TP7	a	602	-	-	3/24/24/24	-
5	COM	a	604[W]	6	-	3/4/4/4	-
6	F43	a	601[A]	10	-	11/28/185/185	-
6	F43	a	601[W]	1,5	-	8/28/185/185	-
5	COM	A	602[A]	-	-	3/4/4/4	-
6	F43	a	603[W]	1,5	-	11/28/185/185	-
5	COM	A	602[W]	6	-	0/4/4/4	-
4	TP7	A	601[W]	-	-	3/24/24/24	-
6	F43	A	603[A]	10	-	12/28/185/185	-
5	COM	a	604[A]	-	-	4/4/4/4	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603[A]	F43	NI-NA	11.57	2.17	1.89
6	a	601[W]	F43	NI-NA	11.49	2.17	1.89
6	a	603[W]	F43	NI-NA	11.41	2.16	1.89
6	a	601[A]	F43	NI-NA	11.05	2.16	1.89
4	a	602	TP7	OXT-C	4.68	1.36	1.22

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	603[A]	F43	CAB-C3B-C2B	-4.84	108.32	119.00
6	a	603[W]	F43	C3B-C4B-CHC	-4.67	113.40	123.33
6	a	601[W]	F43	C3D-C4D-ND	4.50	109.32	102.34
4	a	602	TP7	C-CA-N	-4.16	101.05	110.17
6	A	603[A]	F43	C3B-C4B-CHC	-4.14	114.51	123.33

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	a	602	TP7	C5-C6-C7-S7
5	A	602[A]	COM	C1-C2-S2-O1S
5	A	602[A]	COM	C1-C2-S2-O2S
5	A	602[A]	COM	C1-C2-S2-O3S
5	a	604[A]	COM	C1-C2-S2-O1S

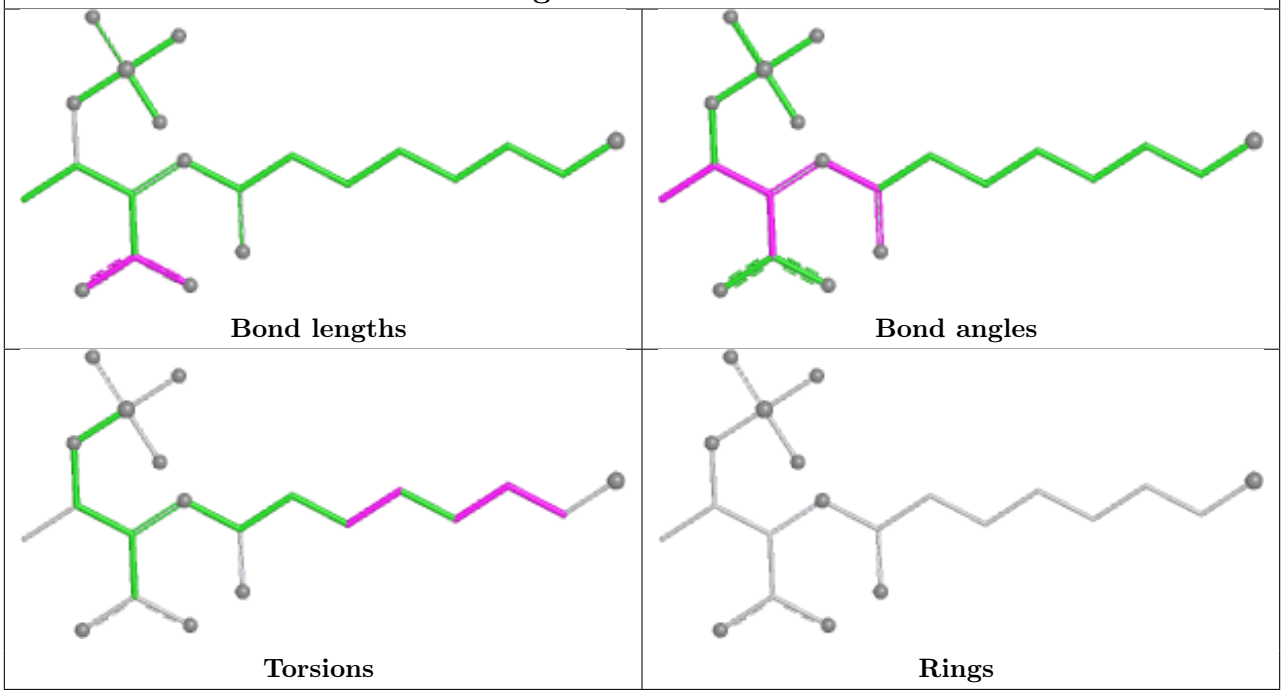
There are no ring outliers.

7 monomers are involved in 20 short contacts:

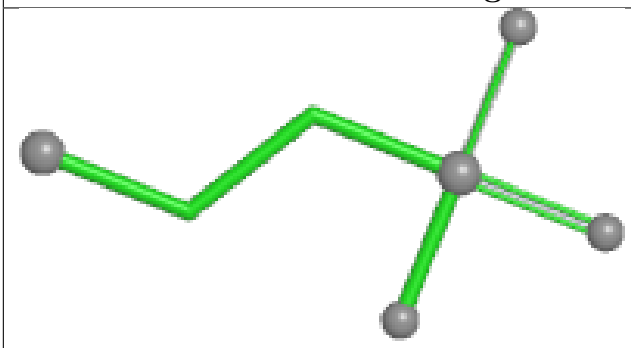
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	602	TP7	4	0
5	a	604[W]	COM	1	0
6	a	601[A]	F43	1	0
6	a	601[W]	F43	1	0
6	a	603[W]	F43	3	0
5	A	602[W]	COM	1	0
6	A	603[A]	F43	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

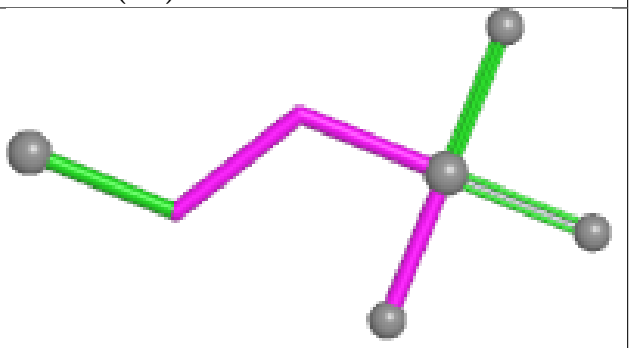
Ligand TP7 a 602



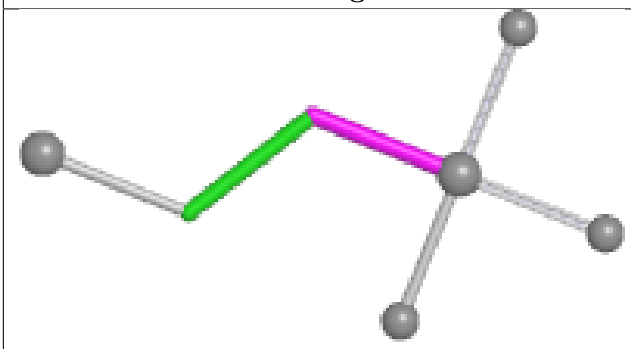
Ligand COM a 604 (W)



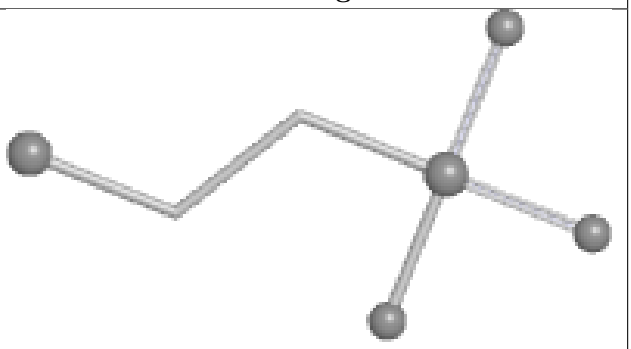
Bond lengths



Bond angles

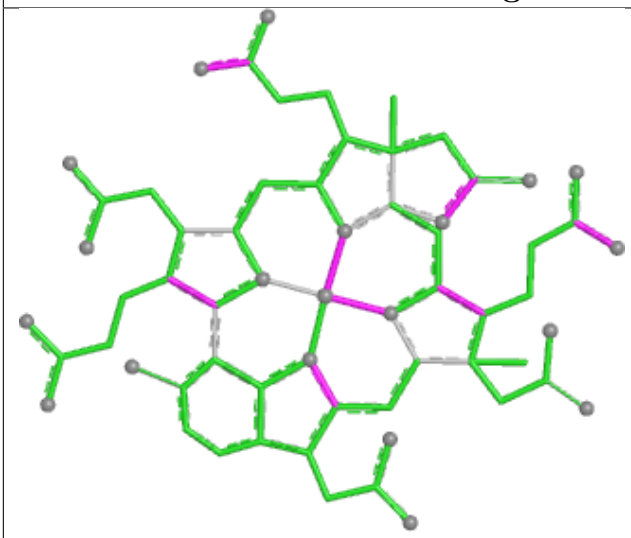


Torsions

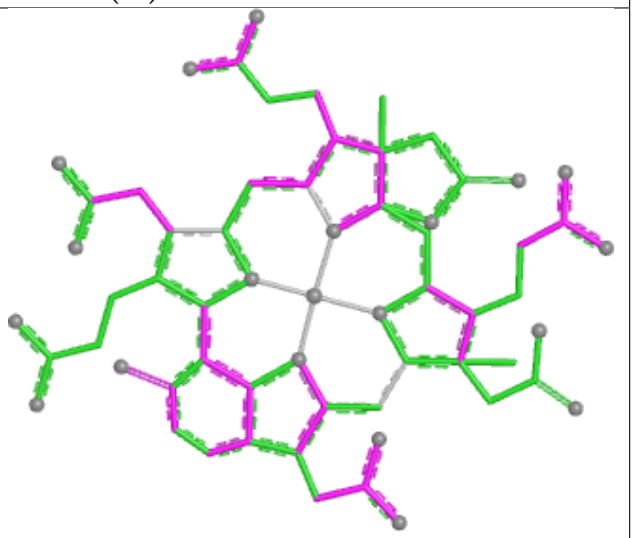


Rings

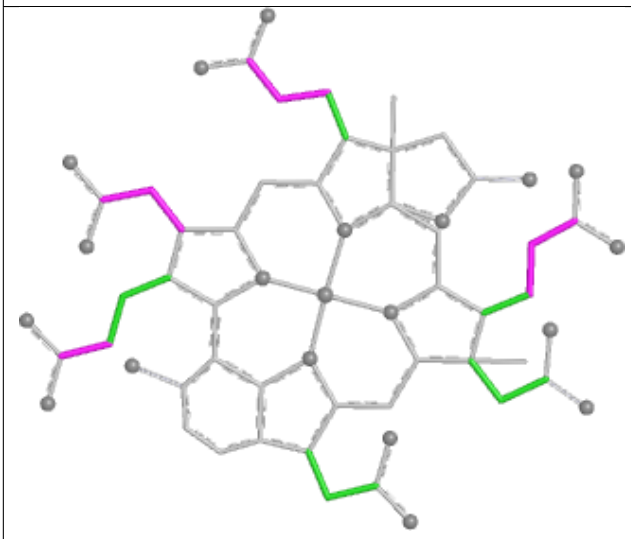
Ligand F43 a 601 (A)



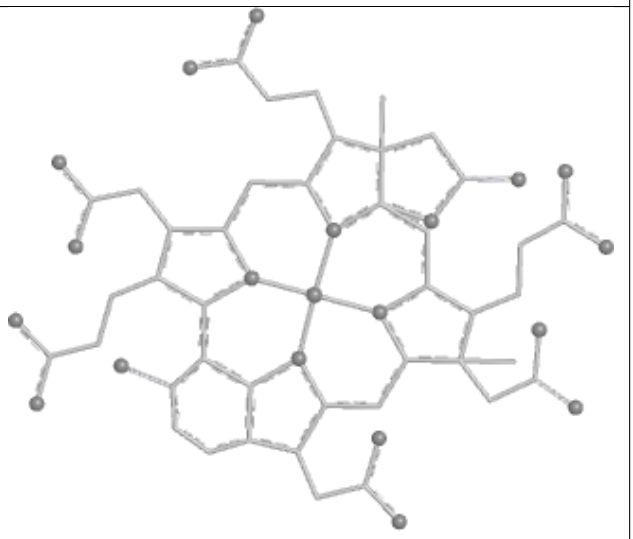
Bond lengths



Bond angles

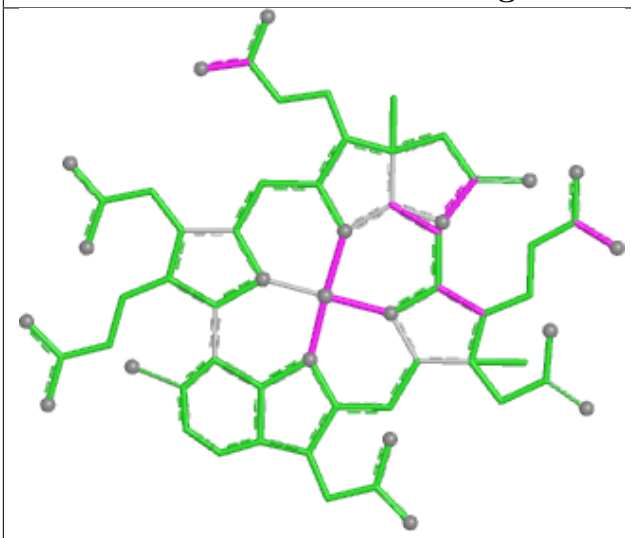


Torsions

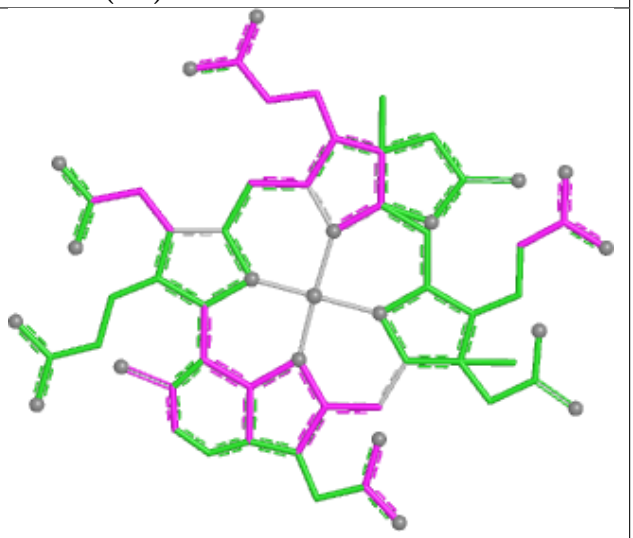


Rings

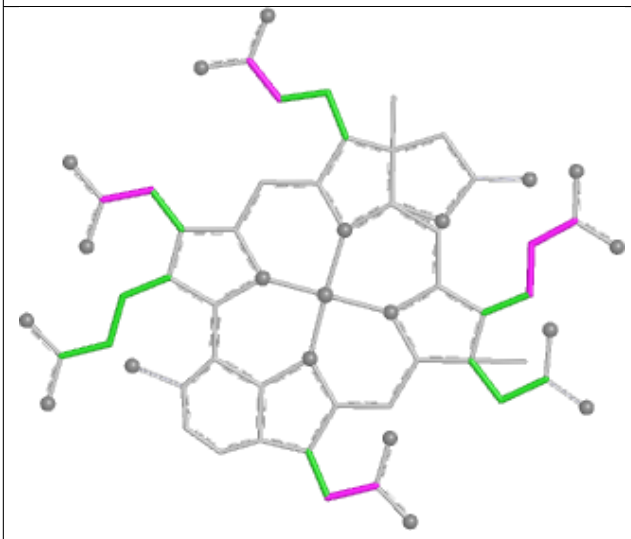
Ligand F43 a 601 (W)



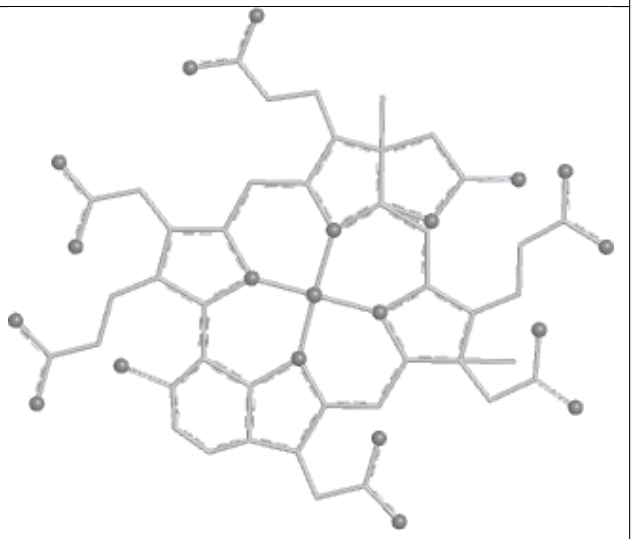
Bond lengths



Bond angles

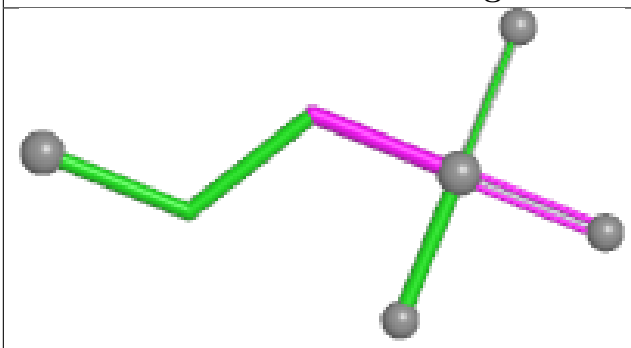


Torsions

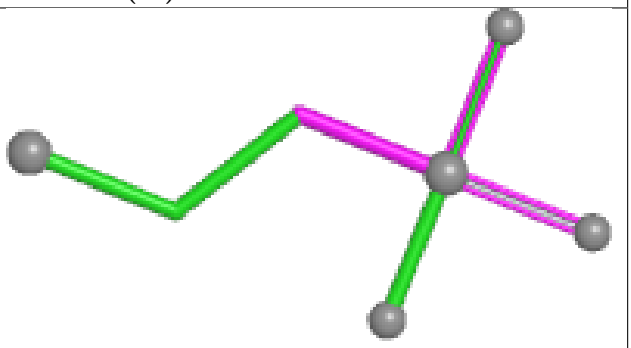


Rings

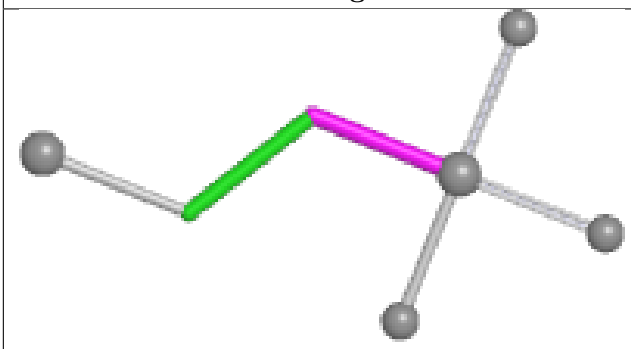
Ligand COM A 602 (A)



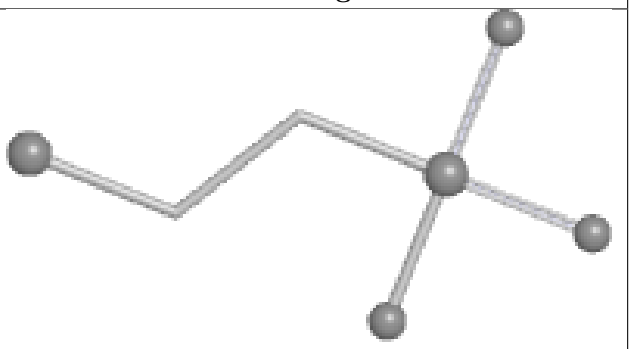
Bond lengths



Bond angles

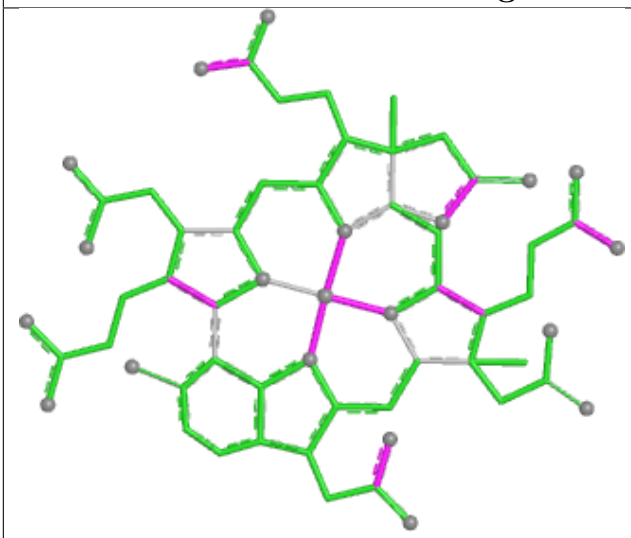


Torsions

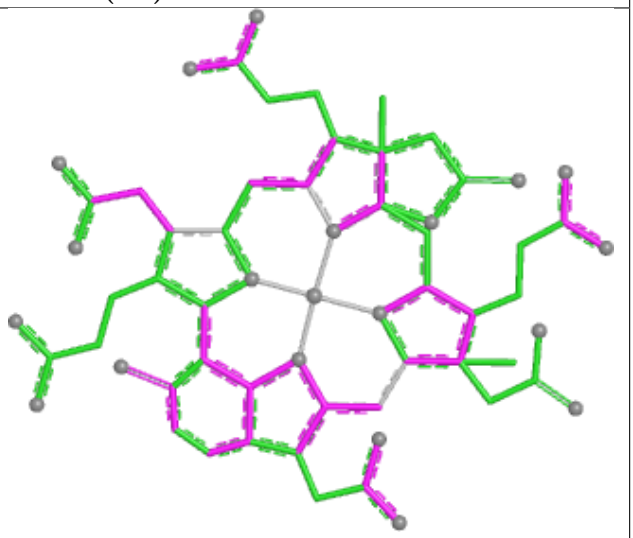


Rings

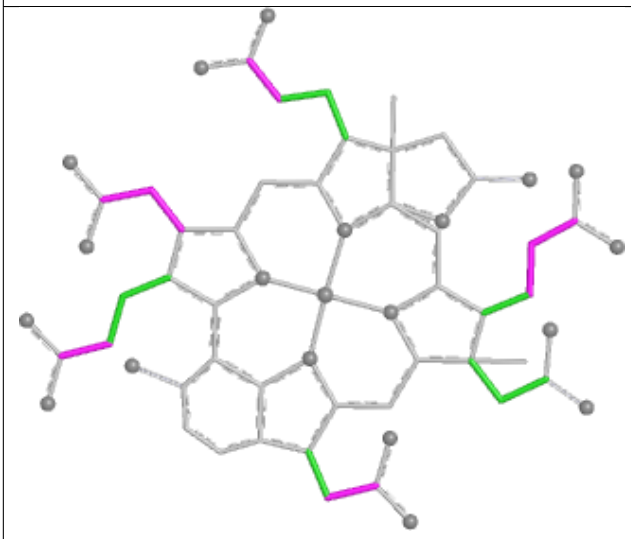
Ligand F43 a 603 (W)



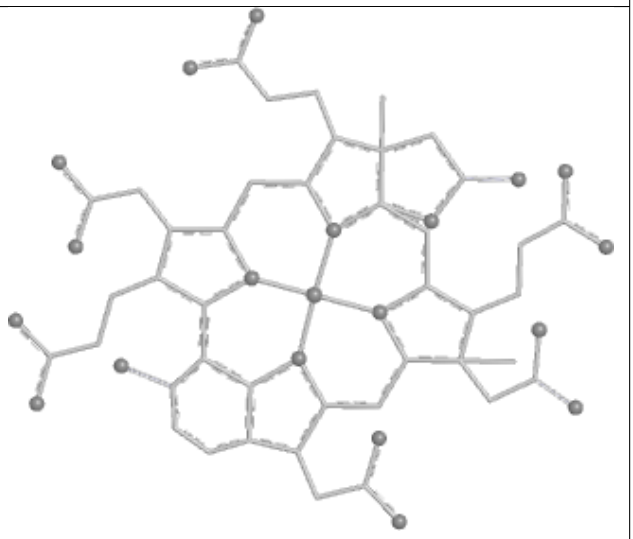
Bond lengths



Bond angles

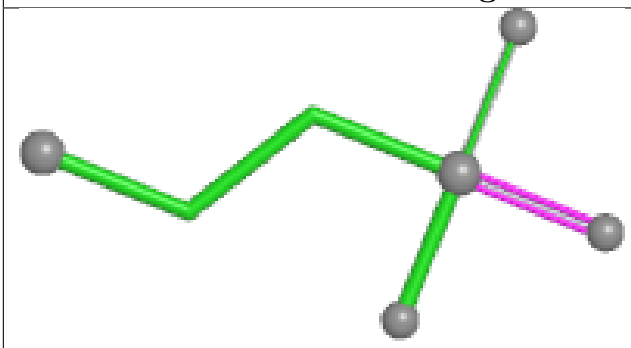


Torsions

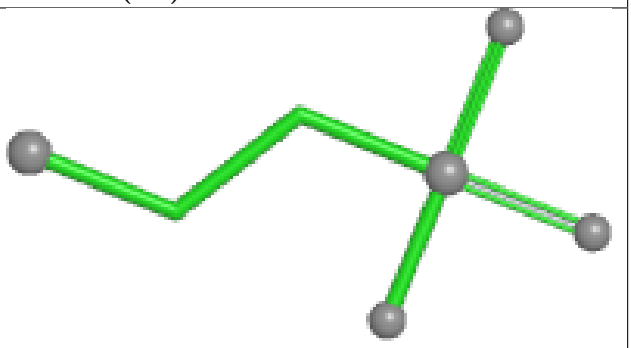


Rings

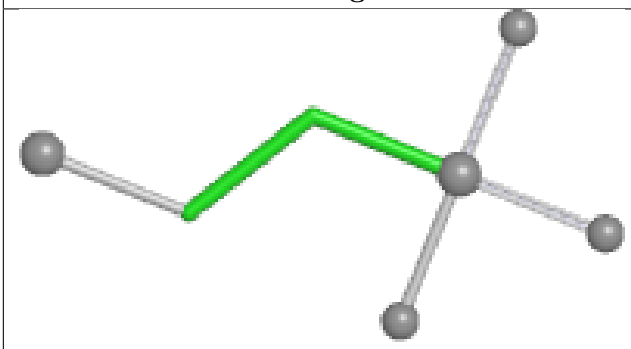
Ligand COM A 602 (W)



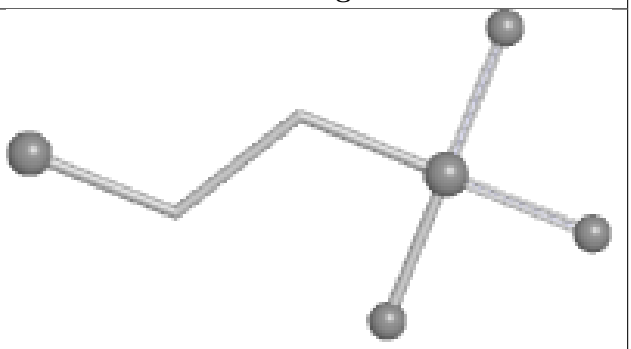
Bond lengths



Bond angles

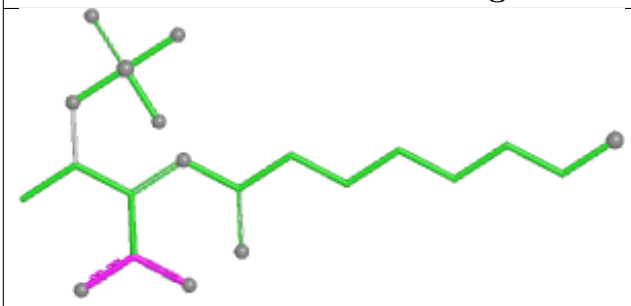


Torsions

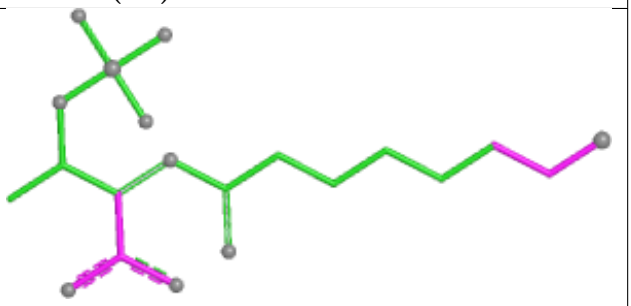


Rings

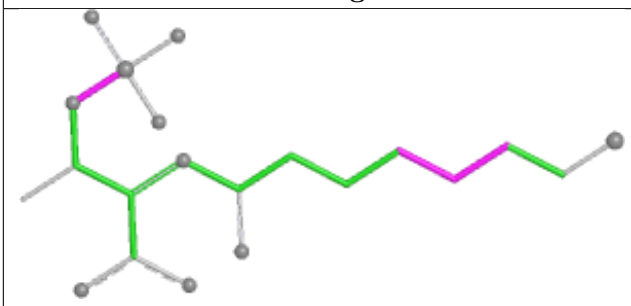
Ligand TP7 A 601 (W)



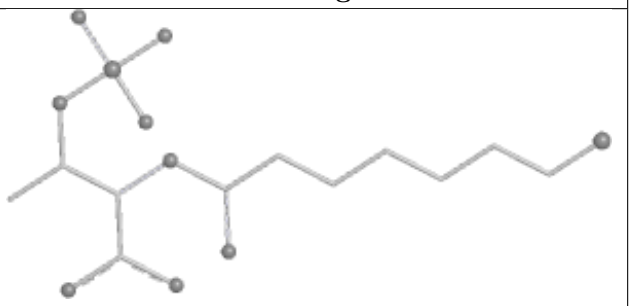
Bond lengths



Bond angles

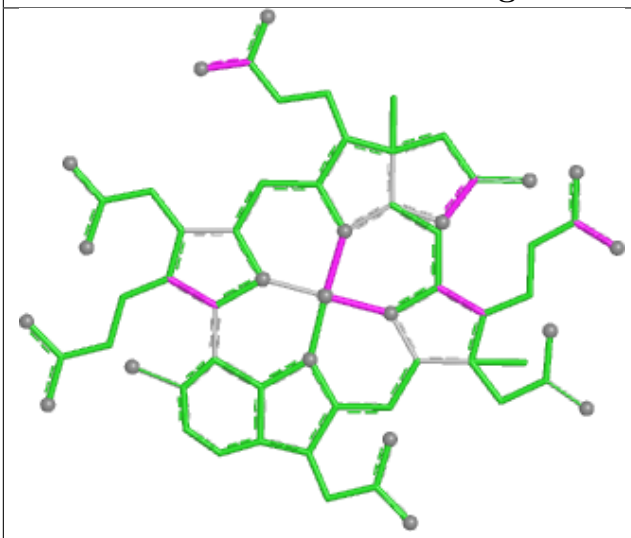


Torsions

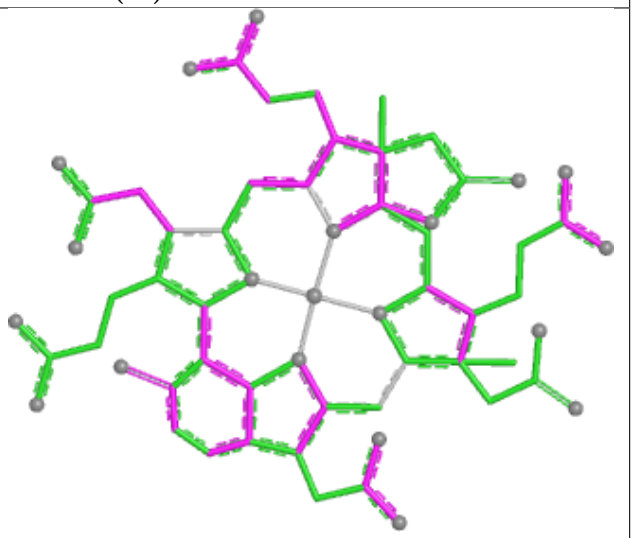


Rings

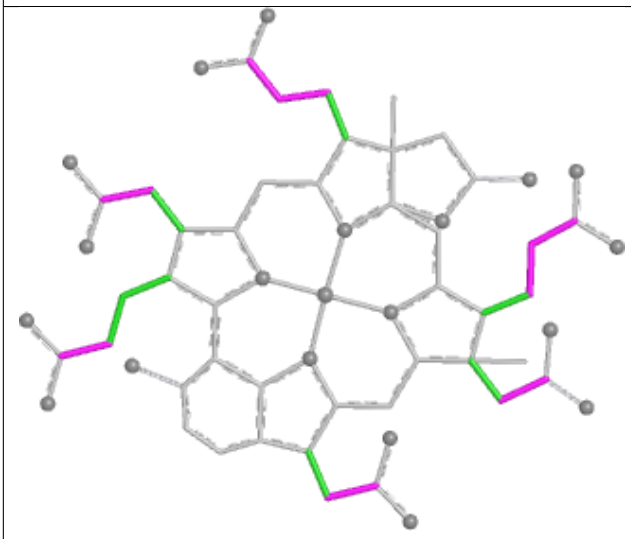
Ligand F43 A 603 (A)



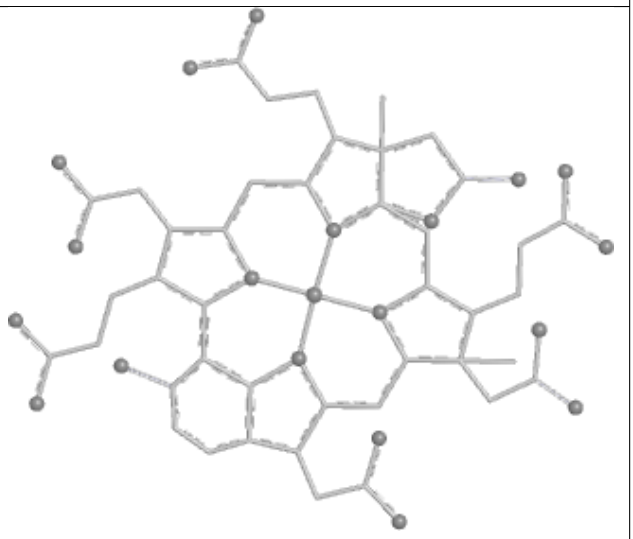
Bond lengths



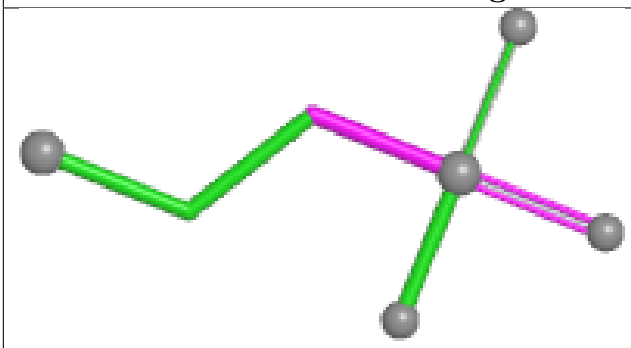
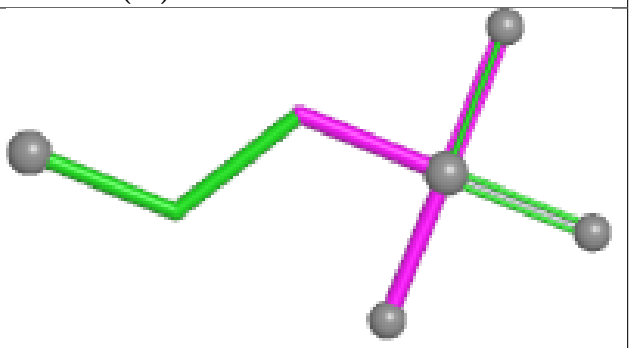
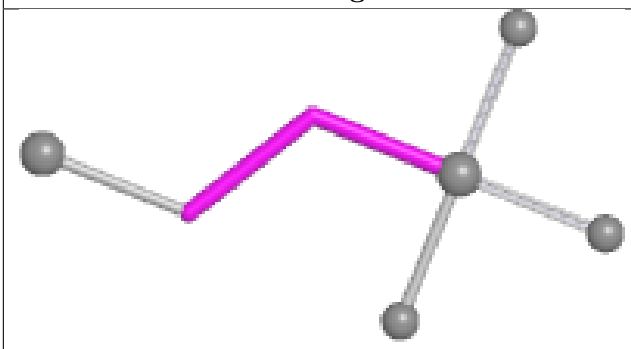
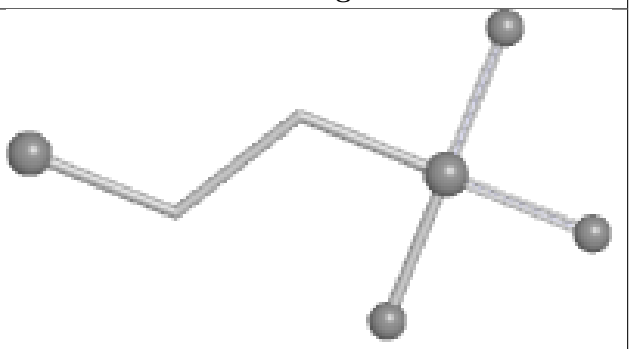
Bond angles



Torsions



Rings

Ligand COM a 604 (A)	
	
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

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	542/548 (98%)	-0.32	5 (0%)	81	86	9, 13, 20, 33	542 (100%)
1	a	542/548 (98%)	-0.37	4 (0%)	84	89	9, 13, 20, 33	542 (100%)
2	B	442/442 (100%)	-0.17	4 (0%)	81	86	10, 15, 21, 29	442 (100%)
2	b	442/442 (100%)	0.08	12 (2%)	56	64	10, 16, 25, 33	442 (100%)
3	C	248/248 (100%)	0.07	5 (2%)	65	73	12, 17, 30, 37	248 (100%)
3	c	248/248 (100%)	0.28	8 (3%)	50	59	12, 20, 31, 41	248 (100%)
All	All	2464/2476 (99%)	-0.13	38 (1%)	72	79	9, 15, 24, 41	2464 (100%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	46[A]	GLY	3.5
2	B	368[A]	GLY	3.2
2	b	413[A]	GLY	3.1
3	C	34[A]	GLU	3.0
2	B	369[A]	GLY	2.9

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	MHS	a	257[A]	11/12	0.92	0.09	23,30,38,38	20
1	MHS	a	257[W]	11/12	0.92	0.09	26,31,37,37	19
1	MHS	A	257[A]	11/12	0.93	0.08	27,31,43,43	19
1	MHS	A	257[W]	11/12	0.93	0.08	25,34,40,40	19

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	AGM	a	271[A]	12/13	0.94	0.07	18,24,29,32	26
1	AGM	a	271[W]	12/13	0.94	0.07	19,23,24,25	26
1	DYA	a	450[A]	8/9	0.96	0.06	19,20,24,26	10
1	DYA	a	450[W]	8/9	0.96	0.06	20,22,25,27	10
1	AGM	A	271[A]	12/13	0.97	0.04	18,24,29,29	26
1	AGM	A	271[W]	12/13	0.97	0.04	17,22,29,30	26
1	MGN	A	400[A]	10/11	0.97	0.05	16,21,23,24	20
1	MGN	A	400[W]	10/11	0.97	0.05	18,22,23,24	20
1	MGN	a	400[A]	10/11	0.97	0.05	18,22,27,27	20
1	MGN	a	400[W]	10/11	0.97	0.05	19,23,27,27	20
1	DYA	A	450[A]	8/9	0.97	0.06	18,21,24,29	10
1	DYA	A	450[W]	8/9	0.97	0.06	19,21,26,28	9
1	SMC	A	452[A]	7/8	0.98	0.04	17,21,26,26	14
1	SMC	A	452[W]	7/8	0.98	0.04	18,21,29,29	14
1	GL3	a	445[A]	4/5	0.99	0.04	22,23,28,28	7
1	GL3	a	445[W]	4/5	0.99	0.04	22,22,29,29	7
1	GL3	A	445[A]	4/5	0.99	0.04	19,20,23,25	7
1	GL3	A	445[W]	4/5	0.99	0.04	18,19,23,23	7
1	SMC	a	452[A]	7/8	0.99	0.04	20,24,31,31	14
1	SMC	a	452[W]	7/8	0.99	0.04	21,23,30,30	13

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	A	609	1/1	0.75	0.19	64,64,64,64	0
8	MG	A	606	1/1	0.82	0.17	74,74,74,74	0
8	MG	A	605	1/1	0.82	0.17	69,69,69,69	0
8	MG	C	301	1/1	0.84	0.16	59,59,59,59	0
8	MG	A	607	1/1	0.86	0.10	59,59,59,59	0
9	NA	C	302	1/1	0.88	0.20	57,57,57,57	0
8	MG	B	501	1/1	0.89	0.08	61,61,61,61	0
8	MG	b	501	1/1	0.90	0.07	62,62,62,62	0

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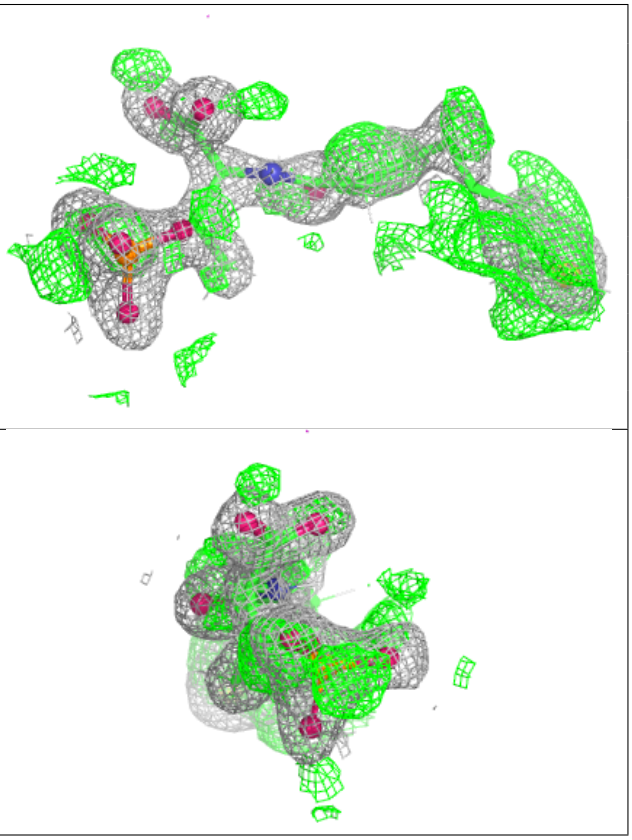
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TP7	A	601[W]	21/21	0.91	0.14	14,24,30,34	40
4	TP7	a	602	21/21	0.92	0.11	21,31,40,46	40
8	MG	A	608	1/1	0.94	0.11	56,56,56,56	0
9	NA	a	607	1/1	0.94	0.08	50,50,50,50	0
9	NA	A	610	1/1	0.95	0.15	40,40,40,40	0
5	COM	A	602[W]	7/7	0.96	0.07	19,23,26,26	11
5	COM	A	602[A]	7/7	0.96	0.07	21,25,30,32	11
5	COM	a	604[W]	7/7	0.97	0.06	21,29,31,31	10
9	NA	a	606	1/1	0.97	0.16	40,40,40,40	0
5	COM	a	604[A]	7/7	0.97	0.06	21,28,32,34	10
6	F43	a	603[W]	62/62	0.98	0.06	16,21,25,30	90
6	F43	A	603[A]	62/62	0.98	0.07	17,21,31,31	89
6	F43	a	601[A]	62/62	0.98	0.06	17,24,29,35	109
6	F43	a	601[W]	62/62	0.98	0.06	18,23,28,33	110
8	MG	a	605	1/1	0.98	0.06	42,42,42,42	0
7	4TI	A	604	1/1	1.00	0.08	28,28,28,28	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.

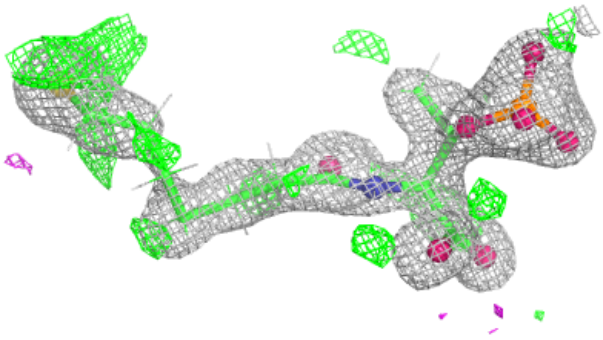
Electron density around TP7 A 601 (W):

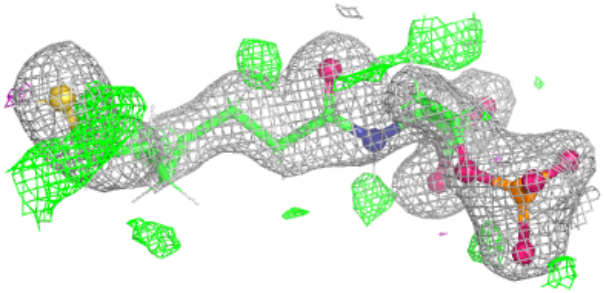
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

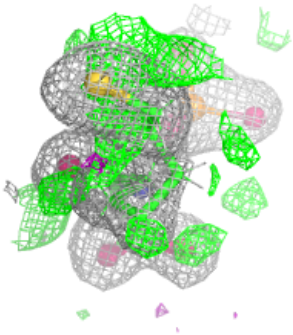


Electron density around TP7 a 602:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

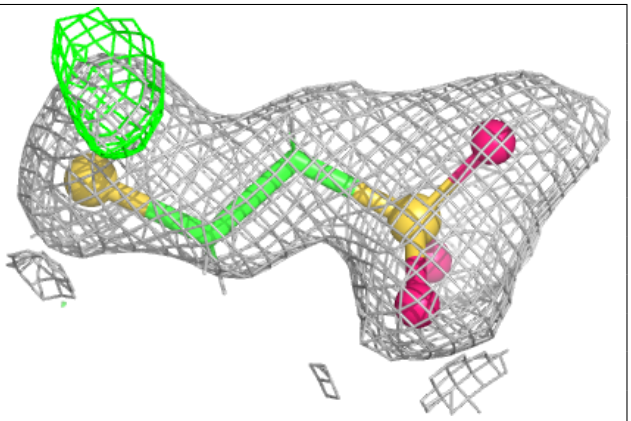


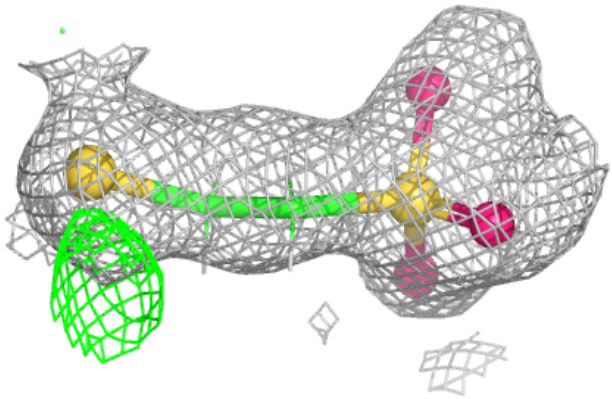


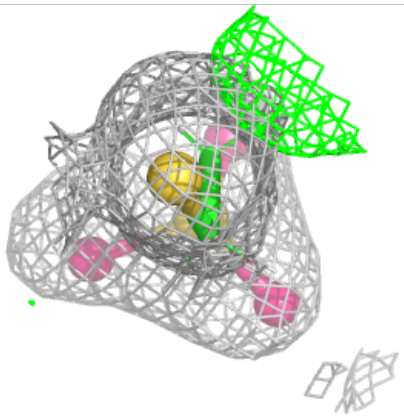


Electron density around COM A 602 (W):

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

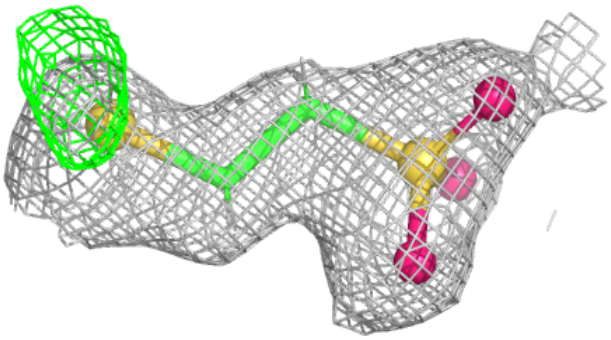


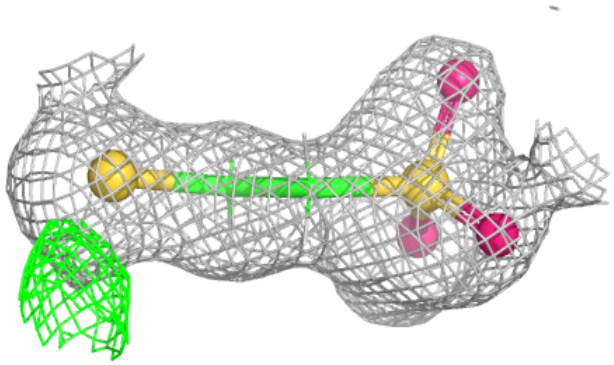


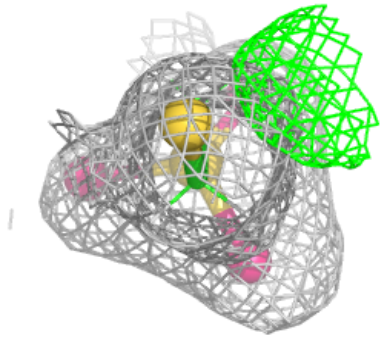


Electron density around COM A 602 (A):

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

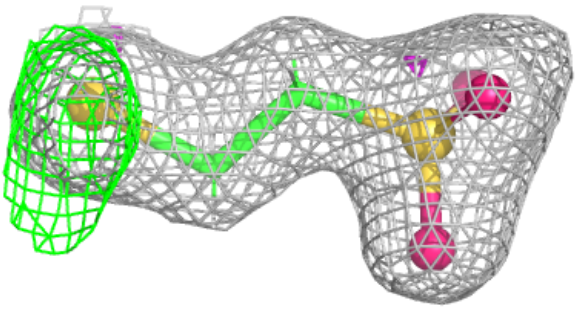


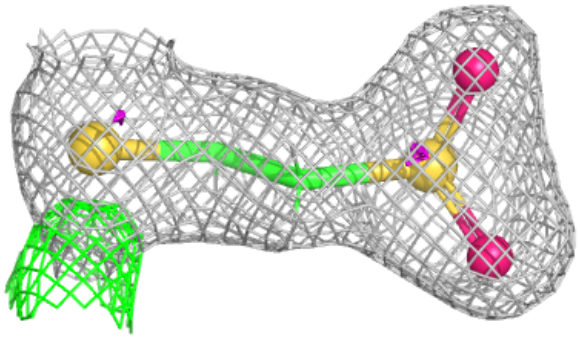


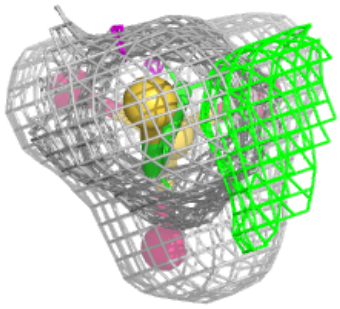


Electron density around COM a 604 (W):

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

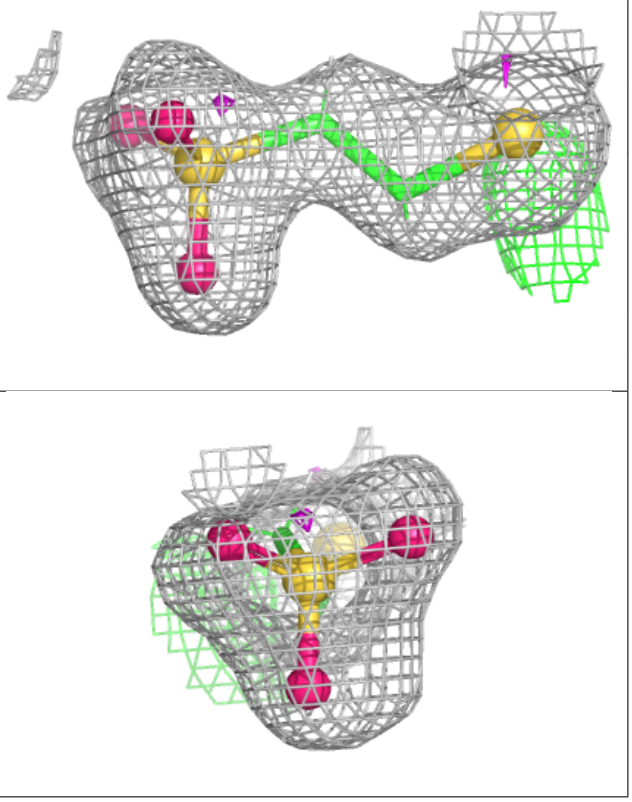






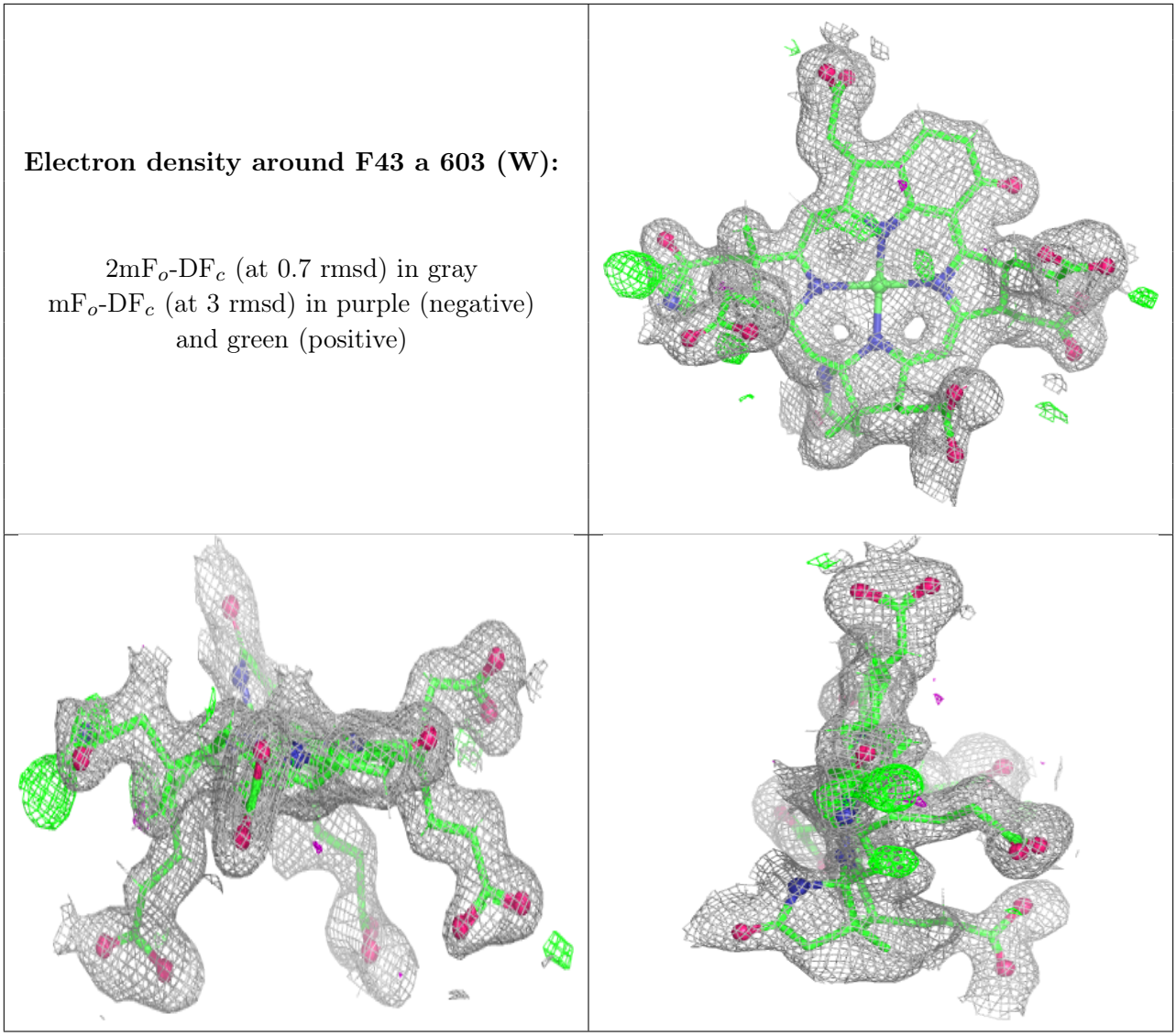
Electron density around COM a 604 (A):

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



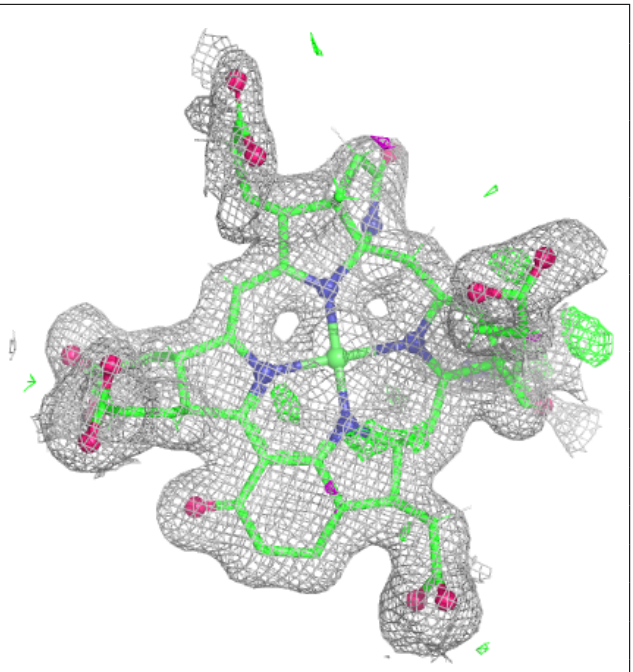
Electron density around F43 a 603 (W):

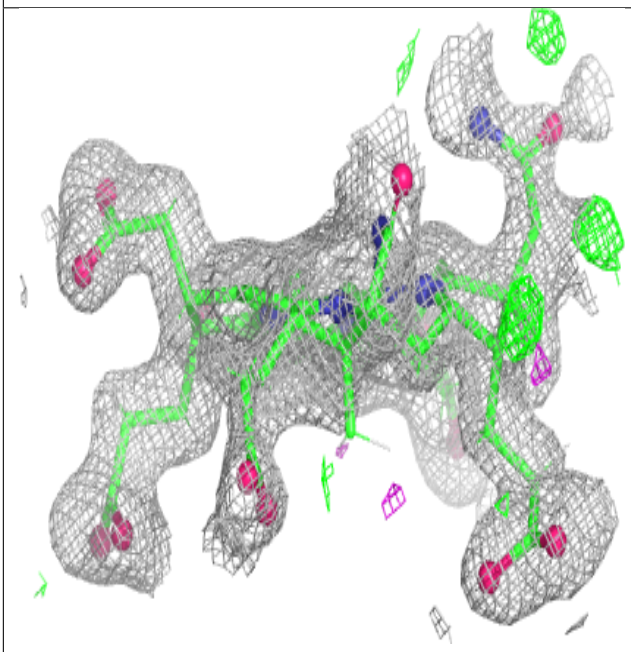
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

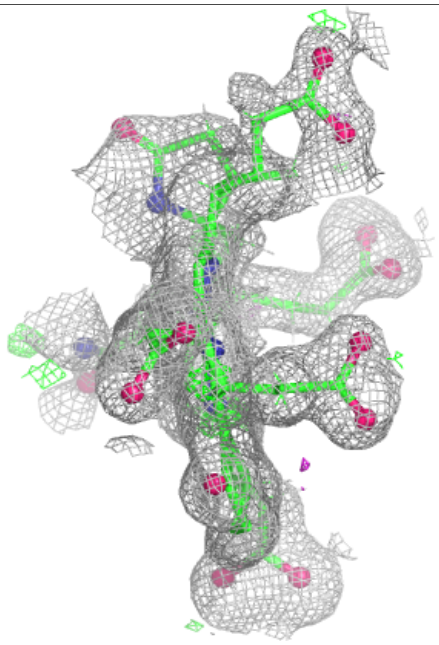


Electron density around F43 A 603 (A):

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

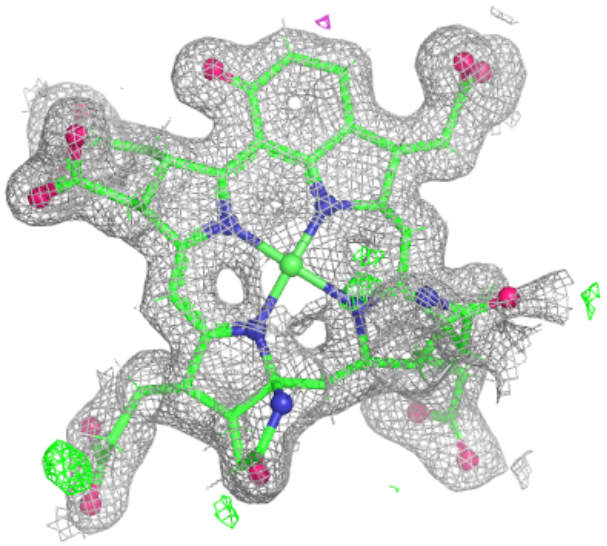


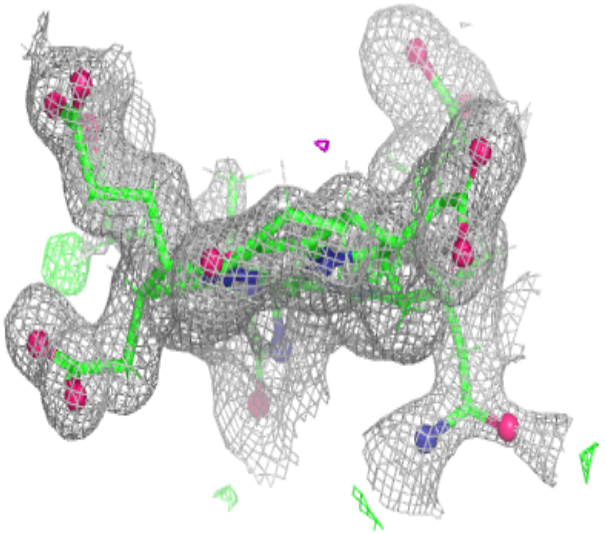


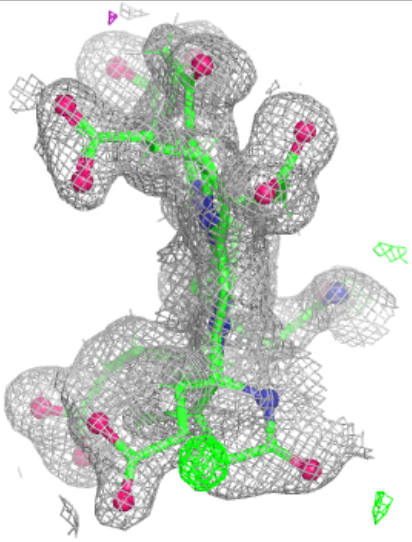


Electron density around F43 a 601 (A):

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

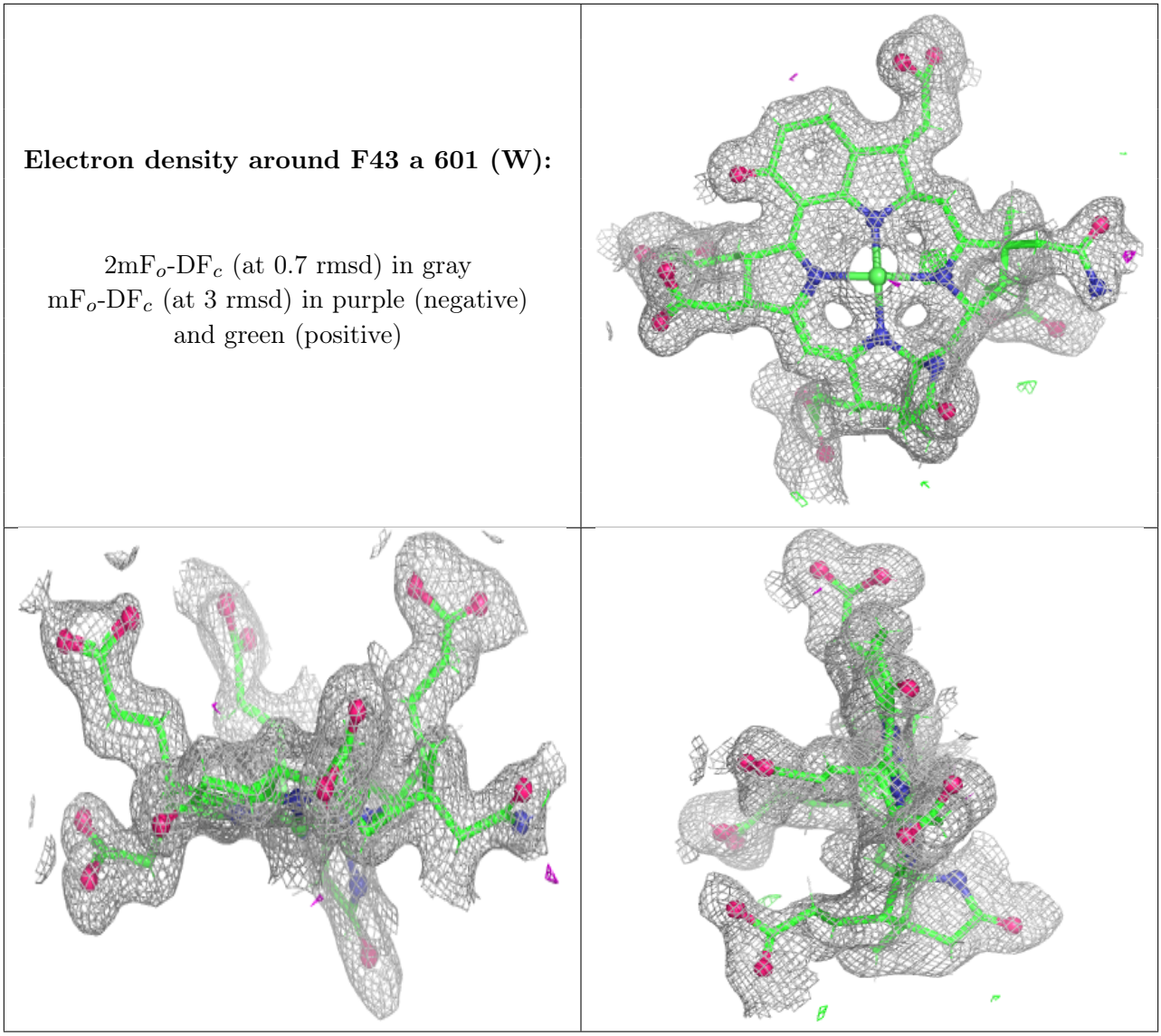






Electron density around F43 a 601 (W):

$2mF_o$-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.