wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2026 – 10:45 AM EDT

PDB ID	:	9MVN / pdb_00009mvn
Title	:	MCRred1-silent
Authors	:	Ohmer, C.J.; Ragsdale, S.W.
Deposited on	:	2025-01-15
Resolution	:	1.50 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:

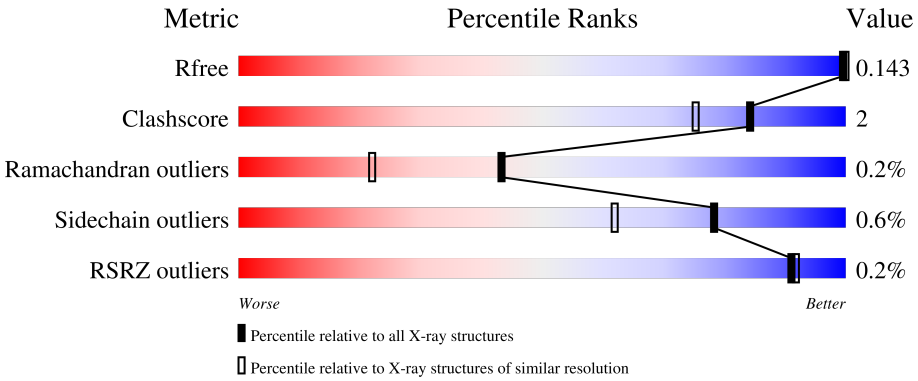
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	550	95% .
1	a	550	94% 5% .
2	B	443	93% 6%
2	b	443	94% 6%
3	C	249	94% 5% .

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Mol	Chain	Length	Quality of chain
3	c	249	94% 5%

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	-	X	-	-
1	DYA	a	450	-	X	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 41156 atoms, of which 19636 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	28	0
			8582	2770	4206	731	854	21			
1	a	548	Total	C	H	N	O	S	0	39	0
			8718	2815	4280	733	868	22			

- 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	30	0
			6930	2187	3481	566	673	23			
2	b	442	Total	C	H	N	O	S	0	31	0
			6937	2191	3481	563	679	23			

- 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	13	0
			4071	1283	2003	359	413	13			
3	c	248	Total	C	H	N	O	S	0	14	0
			4128	1297	2038	365	417	11			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

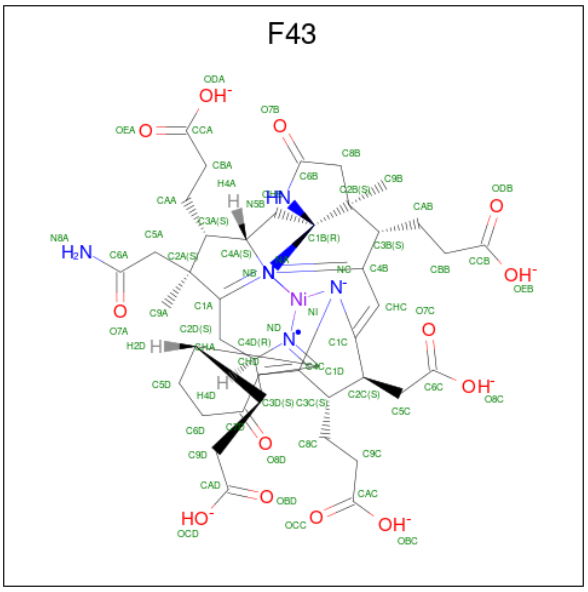
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	a	2	Total	Mg	0	0
			2	2		

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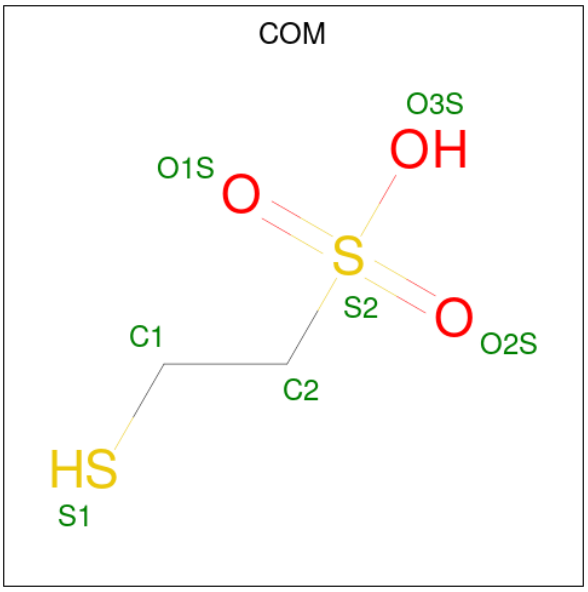
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	b	1	Total Mg 1 1	0	0
4	c	1	Total Mg 1 1	0	0

- Molecule 5 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$) (labeled as "Ligand of Interest" by depositor).



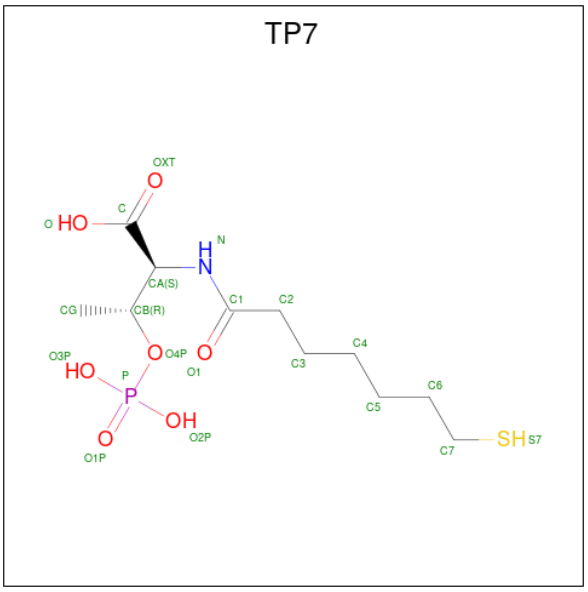
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H N Ni O 110 42 48 6 1 13	0	0
5	a	1	Total C H N Ni O 109 42 47 6 1 13	0	0

- Molecule 6 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
6	A	1	Total	C	H	O	S	0	0
			11	2	4	3	2		
6	a	1	Total	C	H	O	S	0	0
			11	2	4	3	2		

- Molecule 7 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$) (labeled as "Ligand of Interest" by depositor).



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

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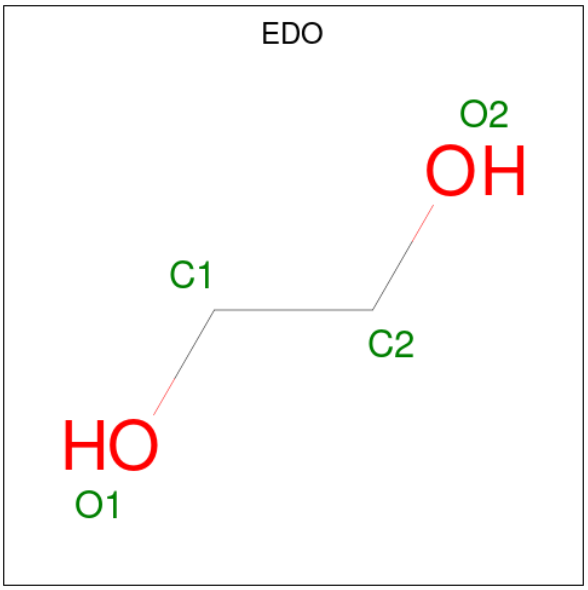
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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	a	1	Total	C	H	N	O	P	S	0	1
			40	11	19	1	7	1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	a	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	a	1	Total	K	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	344	Total	O	0	26
			354	354		

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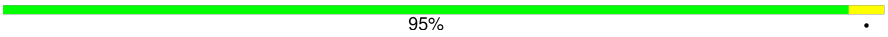
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	238	Total O 242 242	0	9
11	C	141	Total O 144 144	0	3
11	a	343	Total O 357 357	0	28
11	b	210	Total O 213 213	0	6
11	c	134	Total O 139 139	0	6

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

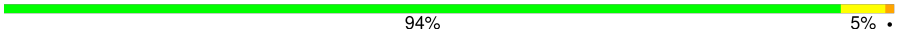
Chain A:

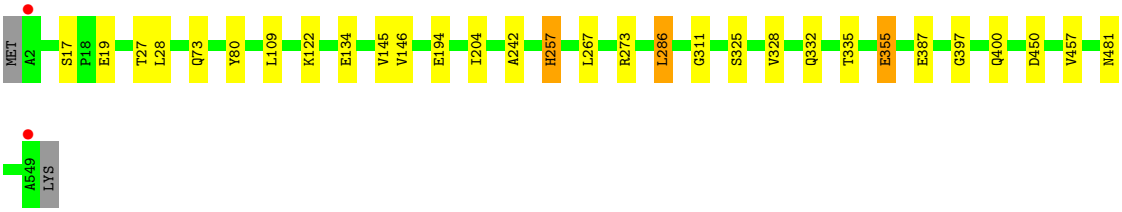




• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

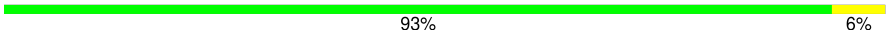
Chain a:

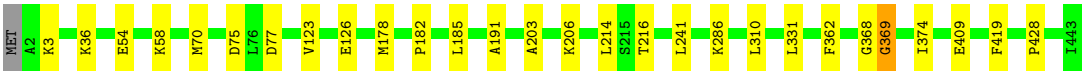




• Molecule 2: Methyl-coenzyme M reductase I subunit beta

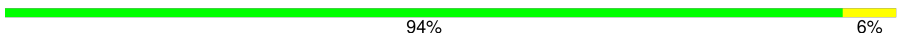
Chain B:

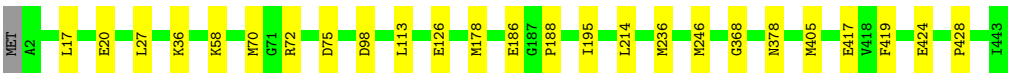




• Molecule 2: Methyl-coenzyme M reductase I subunit beta

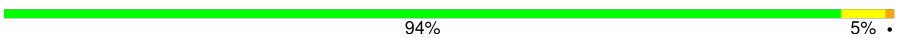
Chain b:





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

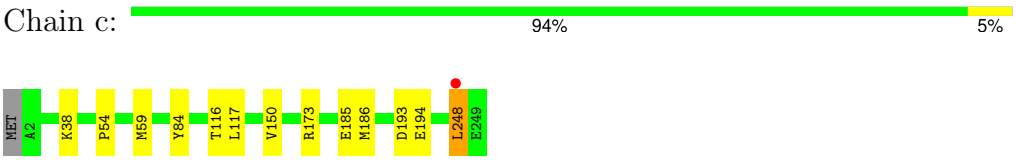
Chain C:





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

Chain c:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.04Å 119.61Å 123.30Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	20.44 – 1.50 20.44 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.44-1.50) 99.9 (20.44-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.50Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.123 , 0.143 0.123 , 0.143	Depositor DCC
R_{free} test set	1803 reflections (0.43%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k 0.012 for -h,-l,-k 0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.99	EDS
Total number of atoms	41156	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: MHS, AGM, DYA, MGN, EDO, SMC, CL, K, TP7, GL3, F43, MG, 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	0.28	0/4515	0.55	0/6129
1	a	0.27	0/4587	0.55	0/6222
2	B	0.25	0/3598	0.52	0/4868
2	b	0.24	0/3619	0.50	0/4896
3	C	0.26	0/2158	0.55	0/2904
3	c	0.25	0/2165	0.54	0/2914
All	All	0.26	0/20642	0.54	0/27933

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	72	ARG	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	4376	4206	4110	17	0
1	a	4438	4280	4187	20	0
2	B	3449	3481	3396	22	0
2	b	3456	3481	3402	18	0
3	C	2068	2003	1967	9	0
3	c	2090	2038	2024	10	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	a	2	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
5	A	62	48	44	2	0
5	a	62	47	44	1	0
6	A	7	4	5	1	0
6	a	7	4	5	0	0
7	A	21	19	19	1	0
7	a	21	19	19	2	0
8	C	1	0	0	0	0
9	a	4	6	6	0	0
10	a	1	0	0	0	0
11	A	354	0	0	6	1
11	B	242	0	0	5	1
11	C	144	0	0	4	0
11	a	357	0	0	6	0
11	b	213	0	0	3	0
11	c	139	0	0	6	0
All	All	21520	19636	19228	91	1

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 2.

The worst 5 of 91 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:259[B]:GLU:OE1	11:A:701[B]:HOH:O	1.79	0.98
3:c:173[B]:ARG:NH1	11:c:401:HOH:O	1.99	0.90
1:a:355[B]:GLU:OE1	11:a:701:HOH:O	1.92	0.86
3:C:207:GLU:OE2	11:C:401:HOH:O	1.98	0.81
1:A:191[A]:ASP:OD1	11:A:702:HOH:O	2.00	0.80

All (1) 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)
11:A:1026:HOH:O	11:B:737:HOH:O[2_545]	2.14	0.06

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	568/550 (103%)	550 (97%)	17 (3%)	1 (0%)	43 22
1	a	578/550 (105%)	562 (97%)	15 (3%)	1 (0%)	43 22
2	B	470/443 (106%)	458 (97%)	10 (2%)	2 (0%)	30 12
2	b	471/443 (106%)	465 (99%)	6 (1%)	0	100 100
3	C	259/249 (104%)	251 (97%)	7 (3%)	1 (0%)	30 12
3	c	260/249 (104%)	251 (96%)	9 (4%)	0	100 100
All	All	2606/2484 (105%)	2537 (97%)	64 (2%)	5 (0%)	43 22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	369[A]	GLY
2	B	369[B]	GLY
3	C	248	LEU
1	A	325	SER
1	a	325	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	458/434 (106%)	456 (100%)	2 (0%)	84 71
1	a	465/434 (107%)	461 (99%)	4 (1%)	70 49
2	B	368/342 (108%)	367 (100%)	1 (0%)	86 75
2	b	370/342 (108%)	367 (99%)	3 (1%)	73 54
3	C	228/217 (105%)	225 (99%)	3 (1%)	61 35
3	c	230/217 (106%)	227 (99%)	3 (1%)	61 35
All	All	2119/1986 (107%)	2103 (99%)	16 (1%)	78 54

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	186	MET
3	c	150	VAL
1	a	355[A]	GLU
2	b	424[B]	GLU
1	a	286[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	ASN
1	a	131	HIS
2	b	174	ASN
1	a	437	GLN
2	B	115	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

13 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	257	1	10,11,12	0.79	0	5,14,16	1.00	1 (20%)
1	DYA	A	450	1	6,7,8	2.96	4 (66%)	6,8,10	4.78	2 (33%)
1	SMC	A	452	1	5,6,7	1.01	0	3,6,8	1.54	0
1	MGN	A	400	1	6,9,10	0.53	0	7,12,14	1.03	0
1	AGM	A	271	1	10,11,12	0.62	0	7,13,15	0.93	0
1	SMC	a	452[A]	1	5,6,7	1.09	0	3,6,8	1.41	0
1	GL3	A	445	1	2,3,4	0.69	0	1,2,4	0.19	0
1	MGN	a	400	1	6,9,10	0.71	0	7,12,14	0.81	0
1	MHS	a	257	1	10,11,12	0.84	0	5,14,16	1.28	1 (20%)
1	DYA	a	450	1	6,7,8	2.05	2 (33%)	6,8,10	4.93	5 (83%)
1	AGM	a	271	1	10,11,12	0.69	0	7,13,15	0.86	0
1	GL3	a	445	1	2,3,4	0.93	0	1,2,4	0.05	0
1	SMC	a	452[B]	1	5,6,7	1.04	0	3,6,8	1.38	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	257	1	-	0/5/6/8	0/1/1/1
1	DYA	A	450	1	-	4/4/6/8	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	2/10/11/13	-
1	SMC	a	452[A]	1	-	1/3/5/7	-
1	GL3	A	445	1	-	1/1/1/2	-
1	MGN	a	400	1	-	0/7/9/12	-
1	MHS	a	257	1	-	0/5/6/8	0/1/1/1
1	DYA	a	450	1	-	4/4/6/8	-
1	AGM	a	271	1	-	2/10/11/13	-
1	GL3	a	445	1	-	1/1/1/2	-
1	SMC	a	452[B]	1	-	1/3/5/7	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	DYA	C-CA	4.54	1.52	1.45
1	a	450	DYA	C-CA	4.14	1.52	1.45
1	A	450	DYA	OD1-CG	-3.61	1.21	1.30
1	A	450	DYA	OD2-CG	3.34	1.31	1.23
1	a	450	DYA	O-C	2.58	1.27	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	DYA	O-C-CA	-10.41	112.34	125.39
1	a	450	DYA	O-C-CA	-10.05	112.79	125.39
1	a	450	DYA	CB-CA-N	-5.11	113.96	123.25
1	A	450	DYA	CB-CA-N	-4.89	114.37	123.25
1	a	257	MHS	ND1-CE1-NE2	-2.74	111.31	112.94

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	450	DYA	N-CA-CB-CG
1	A	450	DYA	O-C-CA-CB
1	A	452	SMC	CA-CB-SG-CS
1	a	450	DYA	N-CA-CB-CG
1	a	450	DYA	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	400	MGN	1	0
1	a	400	MGN	1	0
1	a	257	MHS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	F43	A	602	6,1	63,71,71	1.85	8 (12%)	73,118,118	1.71	18 (24%)
7	TP7	a	601[A]	-	19,20,20	1.42	2 (10%)	24,26,26	1.21	3 (12%)
9	EDO	a	606	-	3,3,3	0.25	0	2,2,2	0.37	0
5	F43	a	604	6,1	63,71,71	1.72	8 (12%)	73,118,118	1.83	21 (28%)
6	COM	A	603	5	6,6,6	1.49	1 (16%)	8,8,8	0.68	0
6	COM	a	605	5	6,6,6	1.57	1 (16%)	8,8,8	0.57	0
7	TP7	A	604[A]	-	19,20,20	1.43	2 (10%)	24,26,26	1.29	4 (16%)

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
5	F43	A	602	6,1	-	8/28/185/185	-
7	TP7	a	601[A]	-	-	3/24/24/24	-
9	EDO	a	606	-	-	1/1/1/1	-
5	F43	a	604	6,1	-	8/28/185/185	-
6	COM	A	603	5	-	0/4/4/4	-
6	COM	a	605	5	-	0/4/4/4	-
7	TP7	A	604[A]	-	-	1/24/24/24	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	F43	NI-NA	10.57	2.14	1.89
5	a	604	F43	NI-NA	9.64	2.12	1.89
5	A	602	F43	NI-NB	4.49	2.00	1.89
7	A	604[A]	TP7	OXT-C	4.40	1.35	1.22
7	a	601[A]	TP7	OXT-C	4.32	1.34	1.22

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	604	F43	C2D-C1D-CHD	-4.34	116.47	121.85
5	a	604	F43	C3D-C4D-ND	4.28	108.98	102.34
5	A	602	F43	C2D-C1D-CHD	-3.98	116.91	121.85
5	a	604	F43	C2B-C1B-NB	3.95	107.73	101.86
5	a	604	F43	C3B-C4B-CHC	-3.95	114.92	123.33

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	F43	C3A-CAA-CBA-CCA
5	a	604	F43	C3A-CAA-CBA-CCA
7	a	601[A]	TP7	C1-C2-C3-C4
7	A	604[A]	TP7	C1-C2-C3-C4
5	a	604	F43	CAA-CBA-CCA-OEA

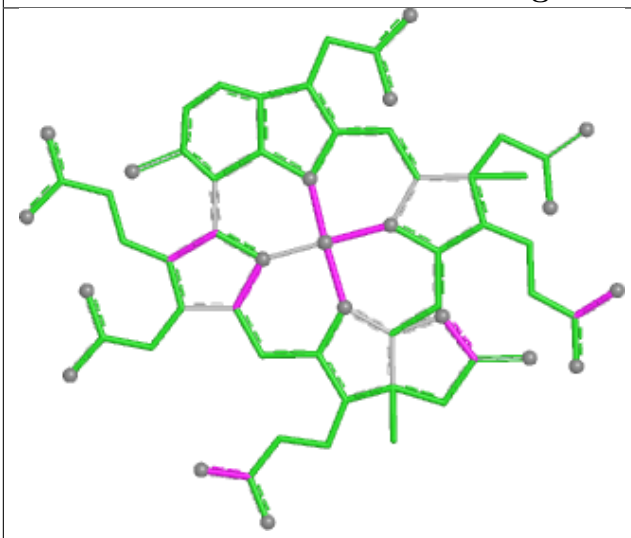
There are no ring outliers.

5 monomers are involved in 7 short contacts:

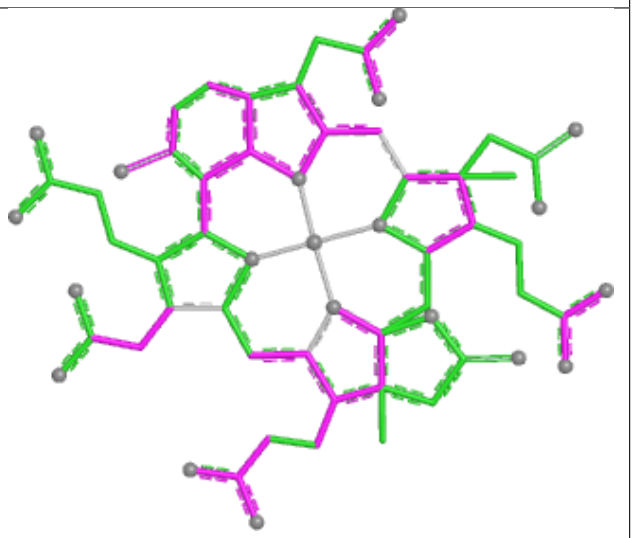
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	F43	2	0
7	a	601[A]	TP7	2	0
5	a	604	F43	1	0
6	A	603	COM	1	0
7	A	604[A]	TP7	1	0

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

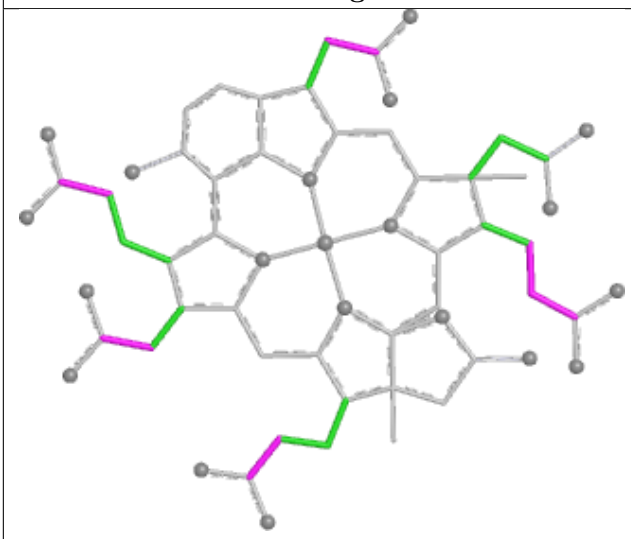
Ligand F43 A 602



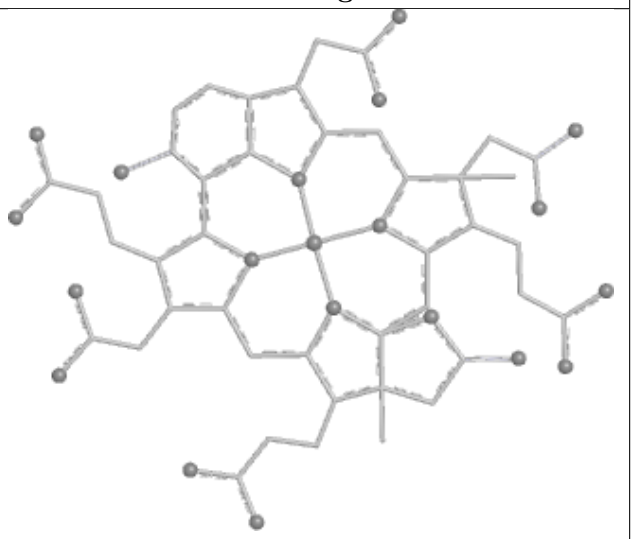
Bond lengths



Bond angles

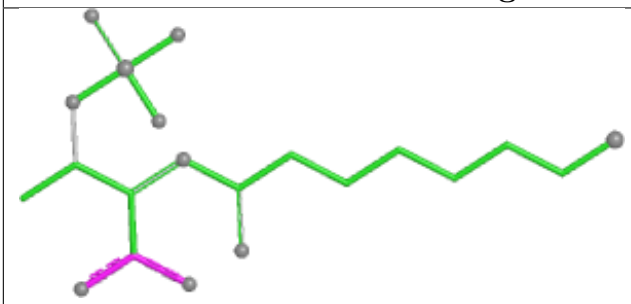


Torsions

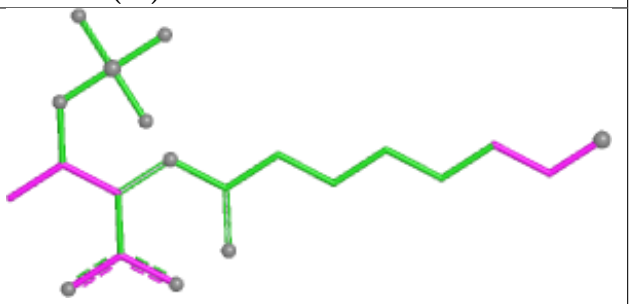


Rings

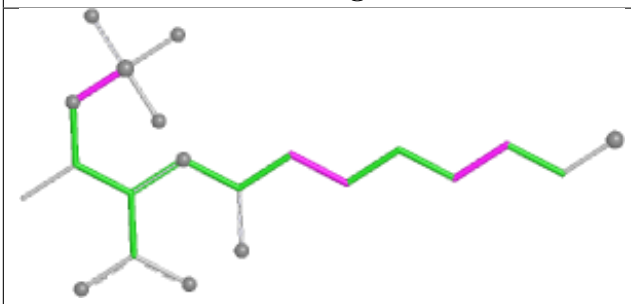
Ligand TP7 a 601 (A)



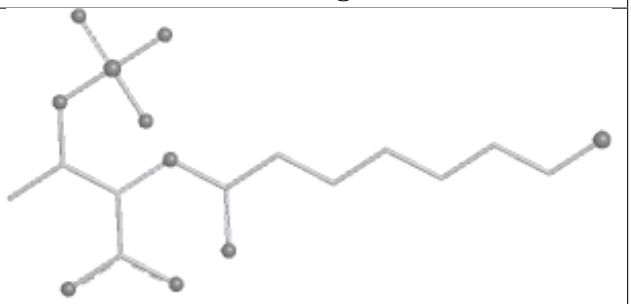
Bond lengths



Bond angles

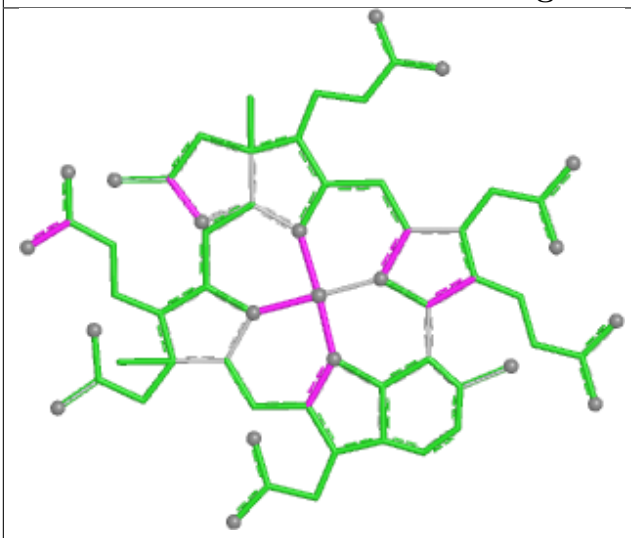


Torsions

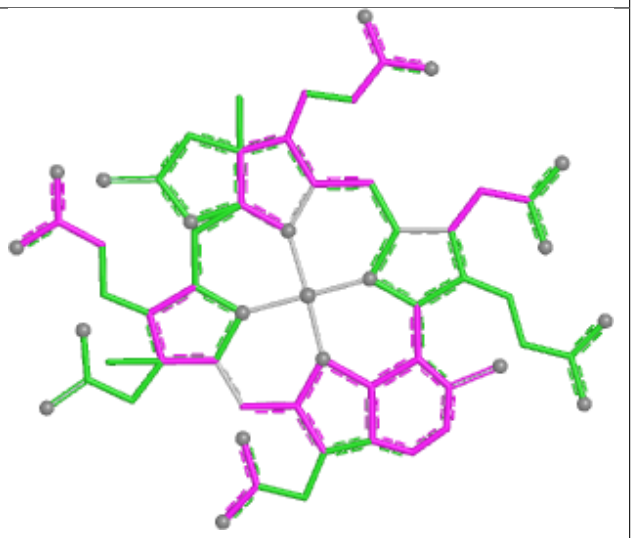


Rings

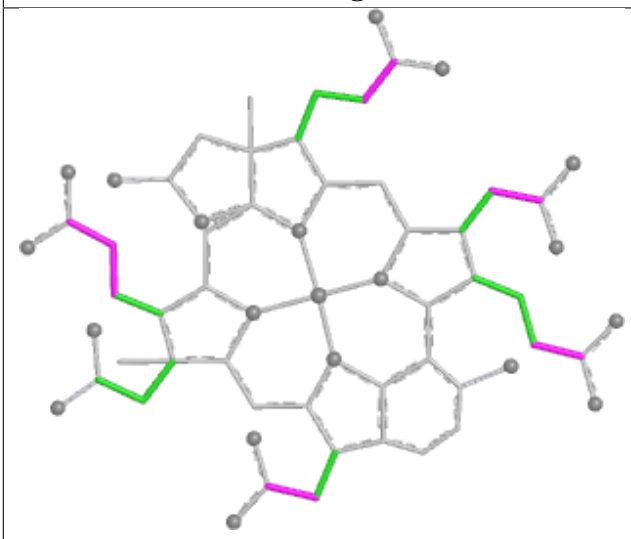
Ligand F43 a 604



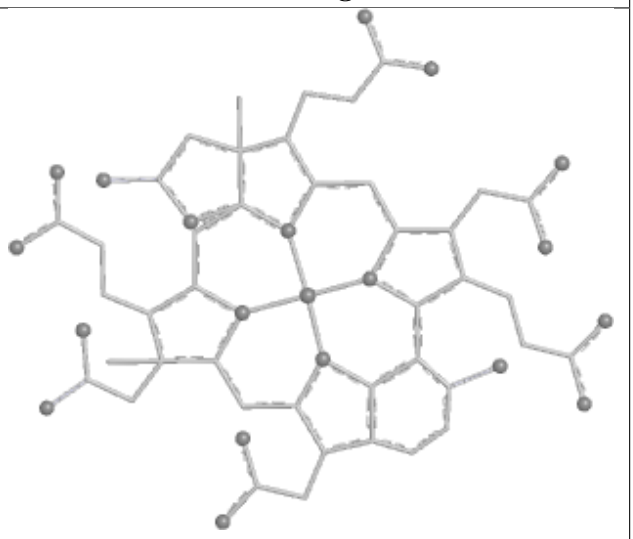
Bond lengths



Bond angles

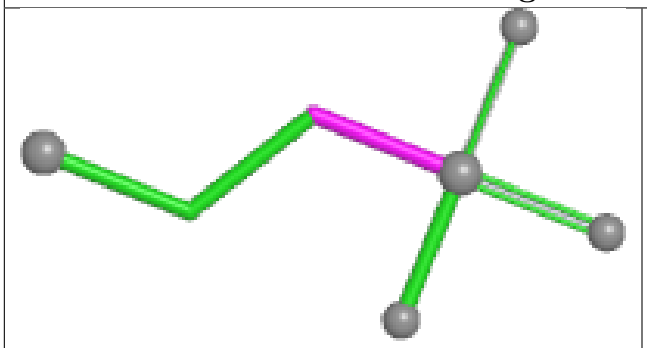


Torsions

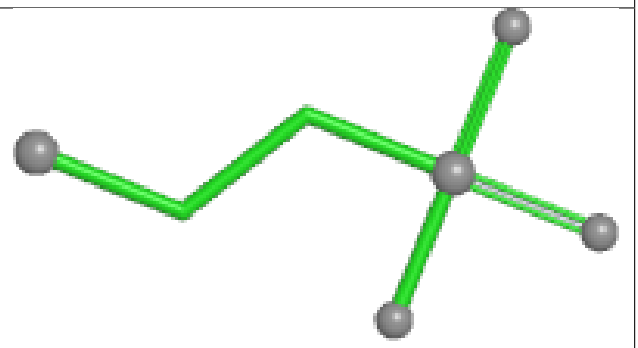


Rings

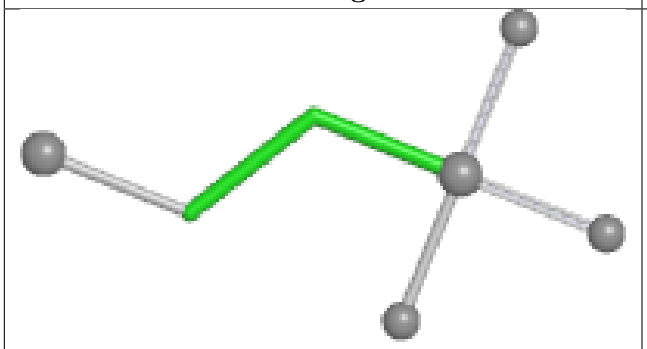
Ligand COM A 603



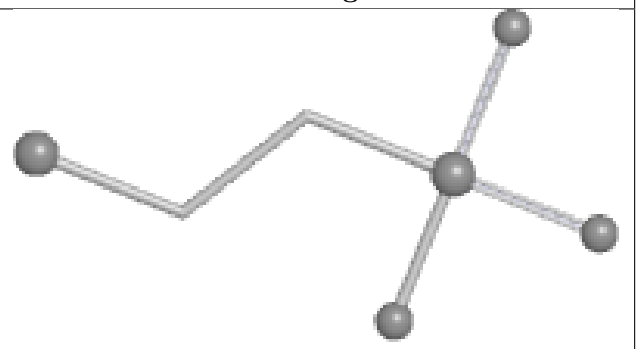
Bond lengths



Bond angles

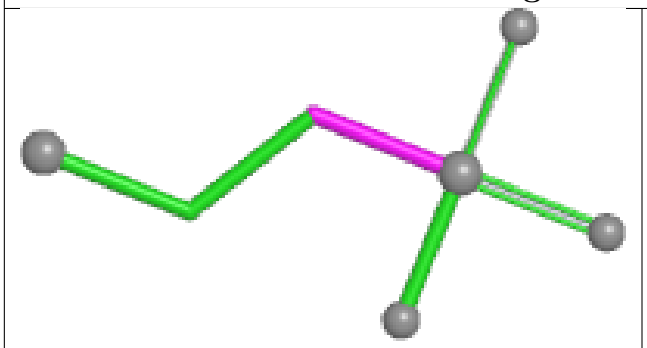


Torsions

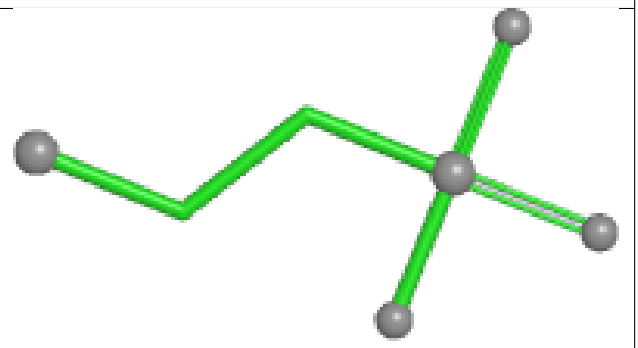


Rings

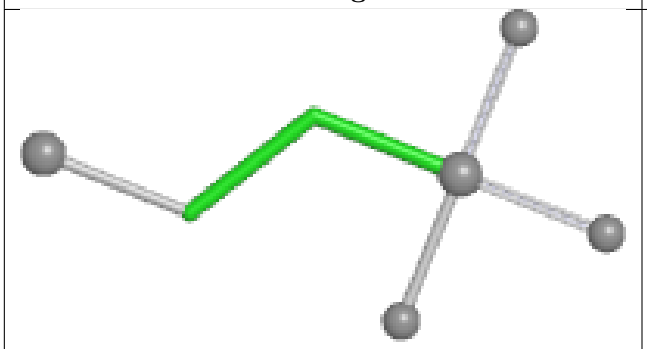
Ligand COM a 605



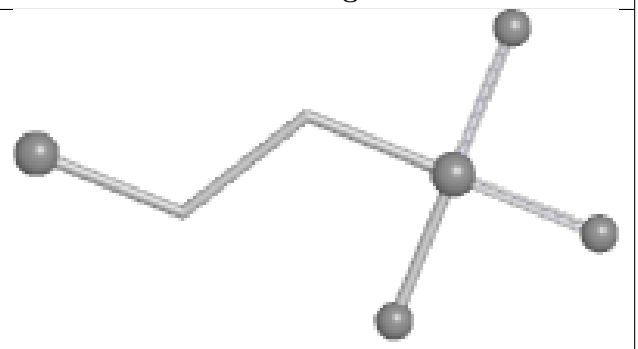
Bond lengths



Bond angles

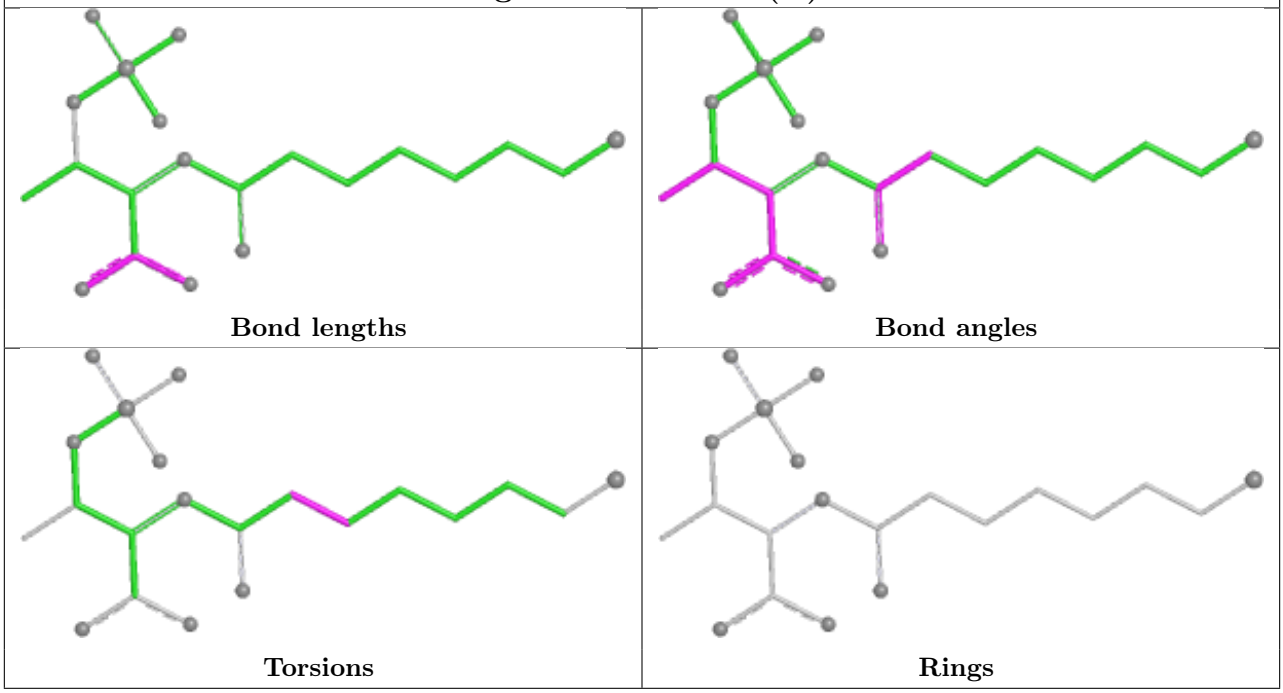


Torsions



Rings

Ligand TP7 A 604 (A)



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	542/550 (98%)	-0.89	0 100 100	10, 24, 44, 88	17 (3%)
1	a	542/550 (98%)	-0.93	2 (0%) 88 90	8, 22, 41, 91	26 (4%)
2	B	442/443 (99%)	-0.71	0 100 100	11, 29, 48, 78	21 (4%)
2	b	442/443 (99%)	-0.58	0 100 100	11, 31, 57, 83	22 (4%)
3	C	248/249 (99%)	-0.57	1 (0%) 88 90	13, 33, 67, 146	9 (3%)
3	c	248/249 (99%)	-0.48	1 (0%) 88 90	15, 35, 63, 149	13 (5%)
All	All	2464/2484 (99%)	-0.74	4 (0%) 91 92	8, 28, 52, 149	108 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	248	LEU	3.9
3	c	248	LEU	3.8
1	a	549	ALA	2.7
1	a	2	ALA	2.4

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	11/12	0.95	0.08	20,31,52,52	0
1	DYA	A	450	8/9	0.96	0.05	17,19,20,21	0
1	MHS	A	257	11/12	0.96	0.07	22,30,48,48	0
1	DYA	a	450	8/9	0.96	0.06	16,16,19,23	0
1	AGM	a	271	12/13	0.98	0.04	15,20,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MGN	A	400	10/11	0.99	0.03	16,20,23,23	0
1	AGM	A	271	12/13	0.99	0.03	14,19,23,23	0
1	MGN	a	400	10/11	0.99	0.03	14,19,22,23	0
1	SMC	A	452	7/8	0.99	0.04	17,21,27,27	0
1	SMC	a	452[A]	7/8	0.99	0.04	16,19,26,26	14
1	SMC	a	452[B]	7/8	0.99	0.04	15,19,23,23	14
1	GL3	a	445	4/5	1.00	0.03	16,18,22,22	0
1	GL3	A	445	4/5	1.00	0.02	15,17,20,20	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

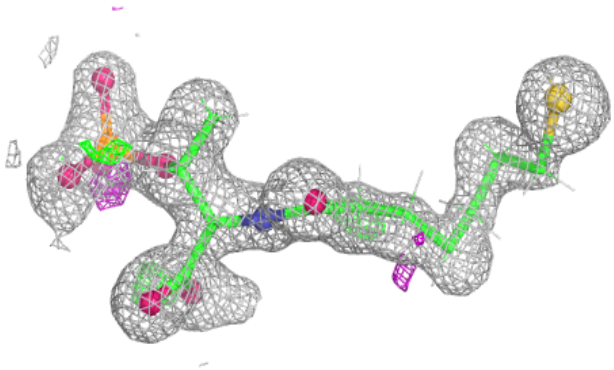
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	a	602	1/1	0.63	0.14	78,78,78,78	0
4	MG	B	502	1/1	0.66	0.15	67,67,67,67	0
9	EDO	a	606	4/4	0.69	0.13	67,81,86,94	0
4	MG	A	601	1/1	0.77	0.12	73,73,73,73	0
4	MG	a	603	1/1	0.78	0.10	79,79,79,79	0
4	MG	B	501	1/1	0.78	0.14	79,79,79,79	0
4	MG	b	501	1/1	0.85	0.10	67,67,67,67	0
8	CL	C	302	1/1	0.89	0.13	42,42,42,42	1
4	MG	c	301	1/1	0.96	0.12	39,39,39,39	0
7	TP7	a	601[A]	21/21	0.98	0.05	14,21,35,35	40
4	MG	C	301	1/1	0.98	0.08	24,24,24,24	1
7	TP7	A	604[A]	21/21	0.98	0.05	14,18,26,30	40
5	F43	A	602	62/62	0.99	0.04	13,18,22,24	0
5	F43	a	604	62/62	0.99	0.04	12,17,22,23	0
6	COM	A	603	7/7	0.99	0.03	15,17,19,19	11
6	COM	a	605	7/7	0.99	0.03	14,17,19,19	11
10	K	a	607	1/1	0.99	0.05	21,21,21,21	0

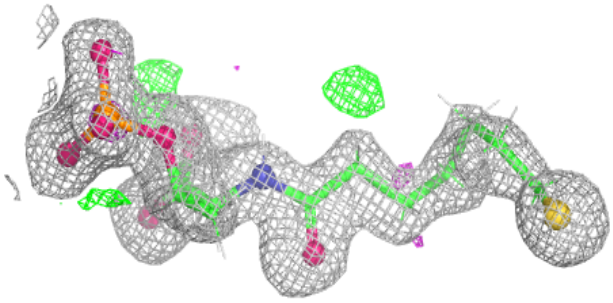
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

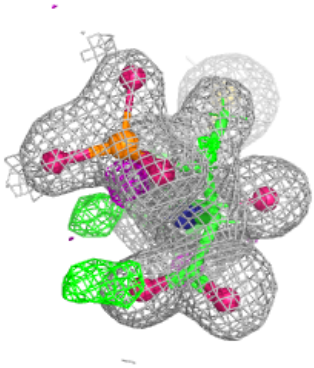
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TP7 a 601 (A):

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

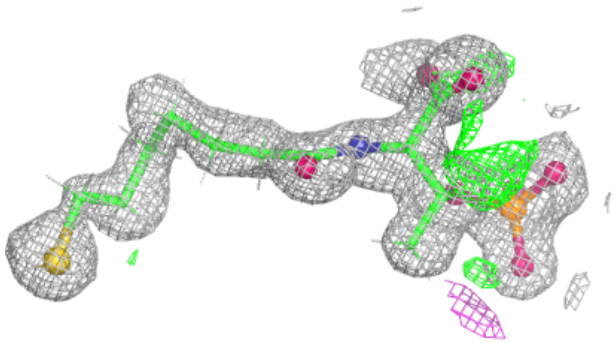


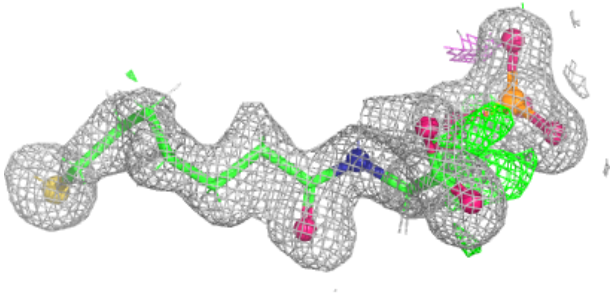


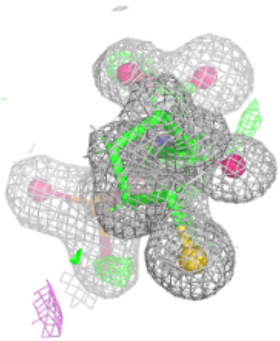


Electron density around TP7 A 604 (A):

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

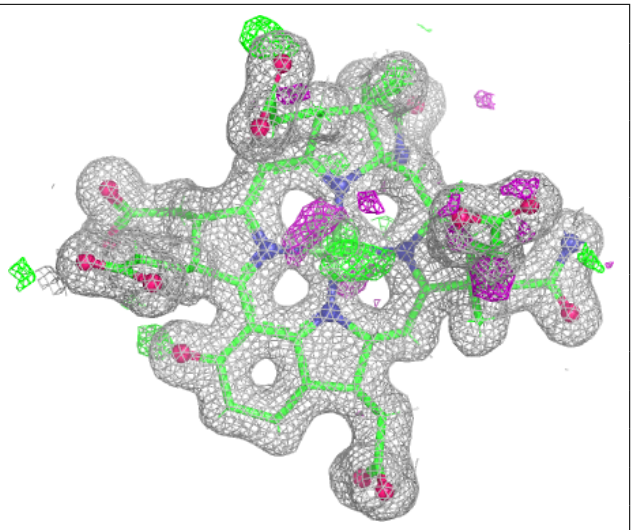


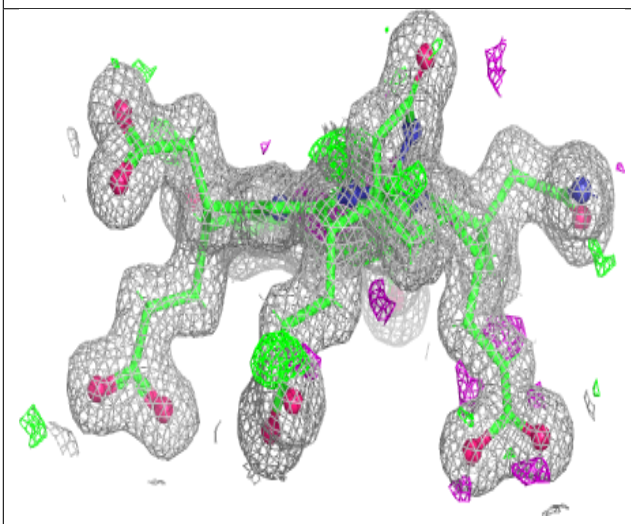


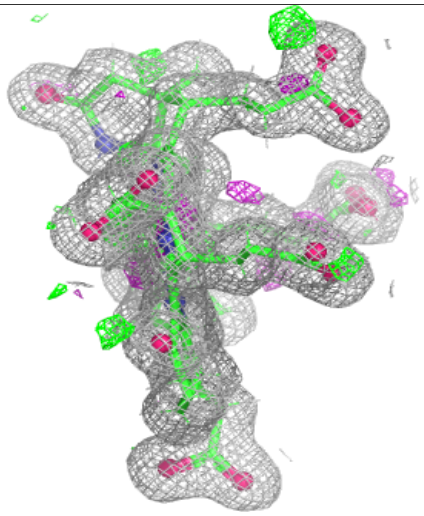


Electron density around F43 A 602:

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

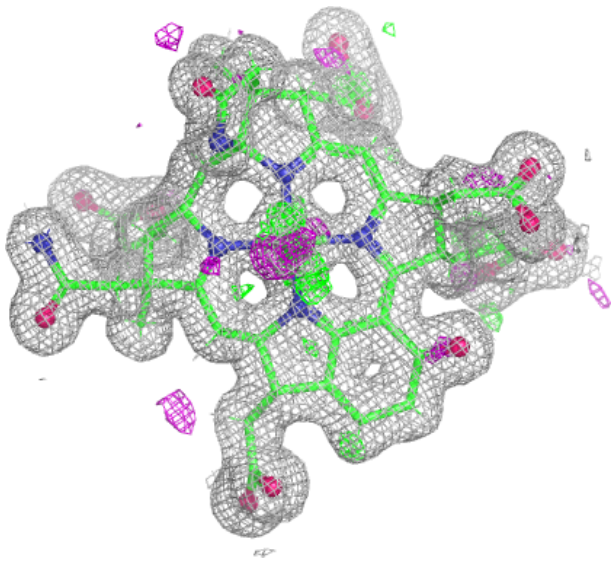


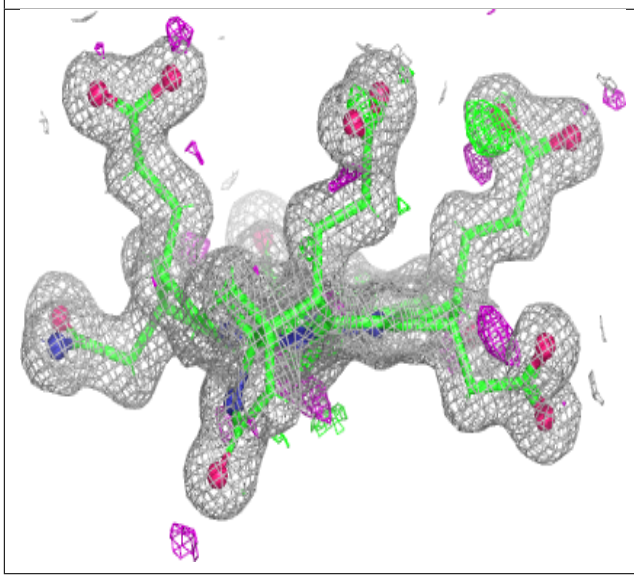


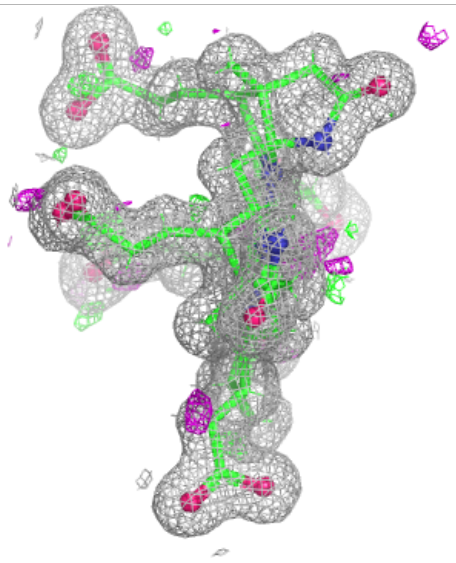


Electron density around F43 a 604:

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

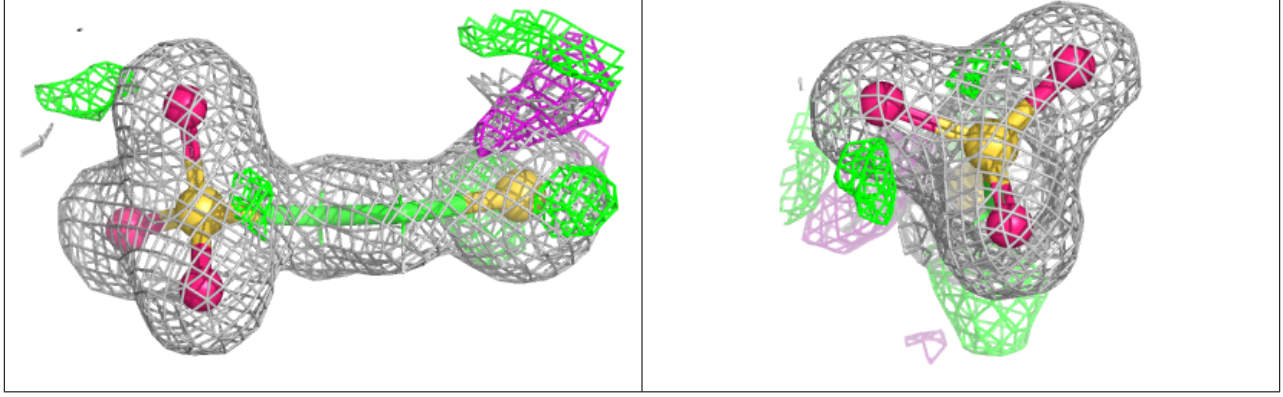






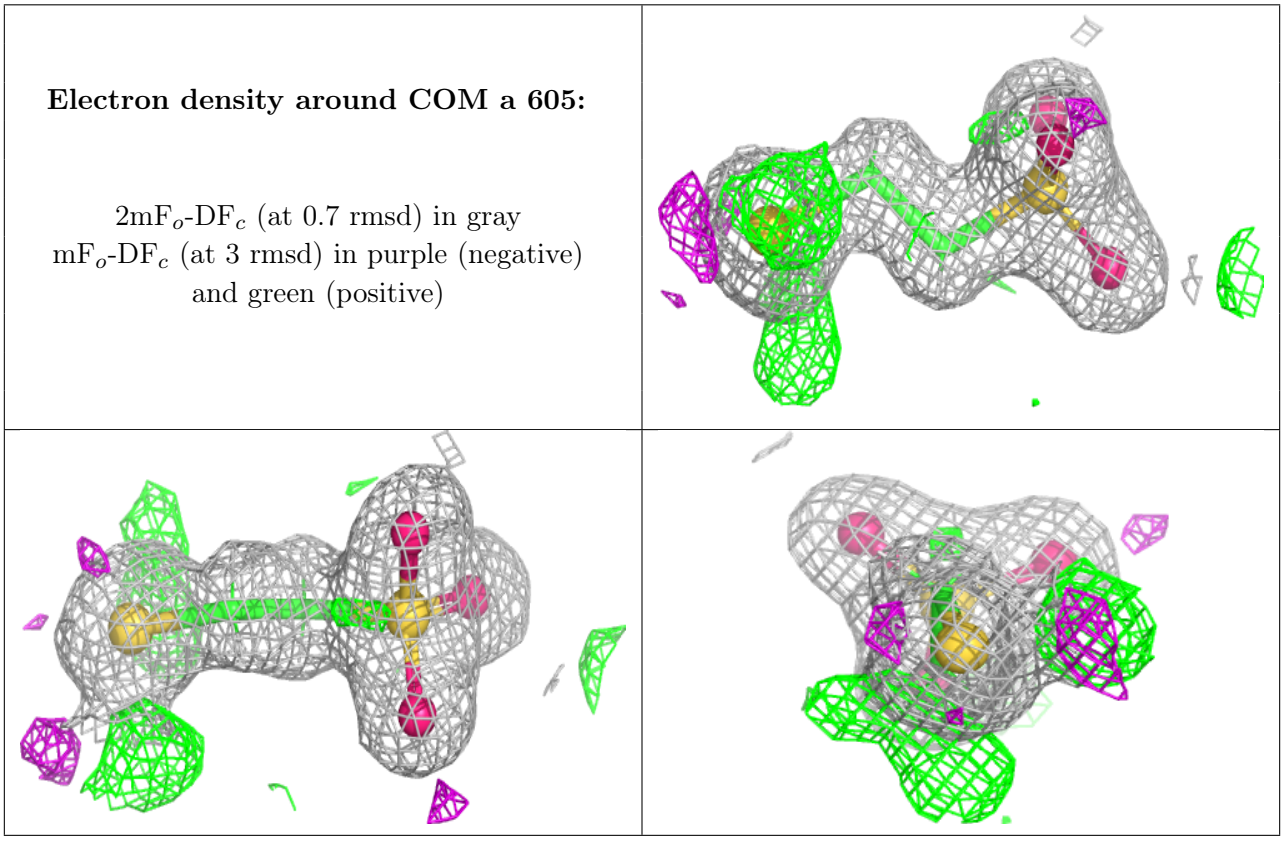
Electron density around COM A 603:

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



Electron density around COM a 605:

$2mF_o$-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.