



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:14 AM UTC

PDB ID : 7B1S / pdb_00007b1s
Title : Crystal structure of the ethyl-coenzyme M reductase from Candidatus
Ethanoperedens thermophilum at 0.994-Å resolution
Authors : Wagner, T.; Lemaire, O.N.; Engilberge, S.
Deposited on : 2020-11-25
Resolution : 0.99 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

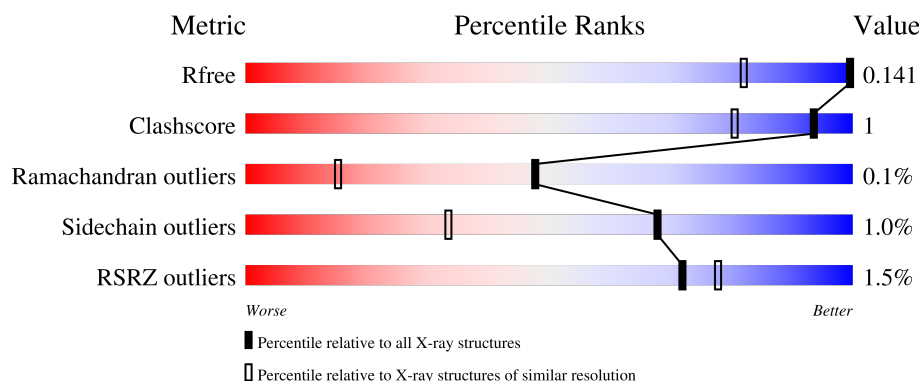
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.99 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.



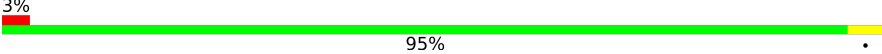
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1358 (1.04-0.96)
Clashscore	190562	1411 (1.04-0.96)
Ramachandran outliers	187476	1347 (1.04-0.96)
Sidechain outliers	187428	1348 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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 $\leq 5\%$. 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	595	% 95% ..
1	D	595	% 95% ..
2	B	467	2% 97% .
2	E	467	% 96% .
3	C	266	3% 97% .

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Mol	Chain	Length	Quality of chain
3	F	266	

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
10	USN	C	301	X	-	-	-
10	USN	D	1101	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25172 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 Ethyl-Coenzyme M reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	33	0
			4862	3061	841	925	35			
1	D	593	Total	C	N	O	S	0	35	0
			4879	3081	846	918	34			

- Molecule 2 is a protein called Ethyl-Coenzyme M reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	33	0
			3737	2367	637	715	18			
2	E	466	Total	C	N	O	S	0	37	0
			3731	2374	630	709	18			

- Molecule 3 is a protein called Ethyl-Coenzyme M reductase gamma subunit.

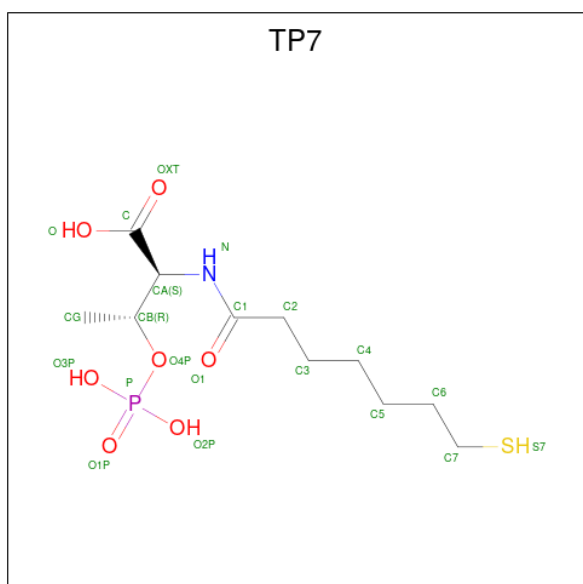
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	23	0
			2299	1427	414	437	21			
3	F	265	Total	C	N	O	S	0	24	0
			2317	1432	416	448	21			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 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
5	A	1	Total	C	N	O	P	S	
			21	11	1	7	1	1	
5	D	1	Total	C	N	O	P	S	
			21	11	1	7	1	1	

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn		
			1	1	0	0

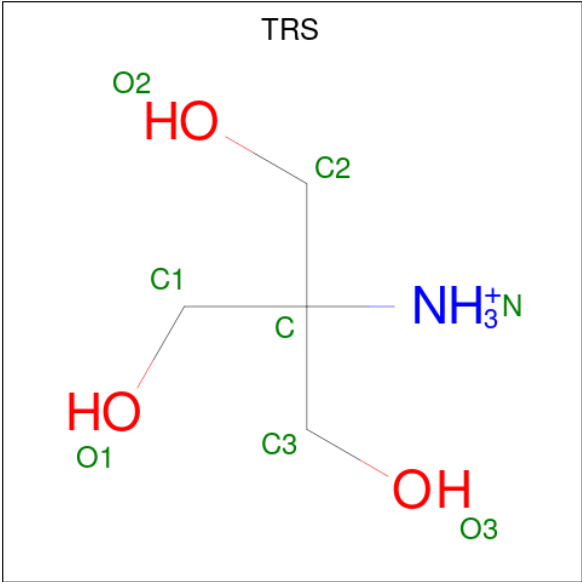
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	K		
			2	2	0	1
7	C	1	Total	K		
			1	1	0	0
7	D	1	Total	K		
			1	1	0	1

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

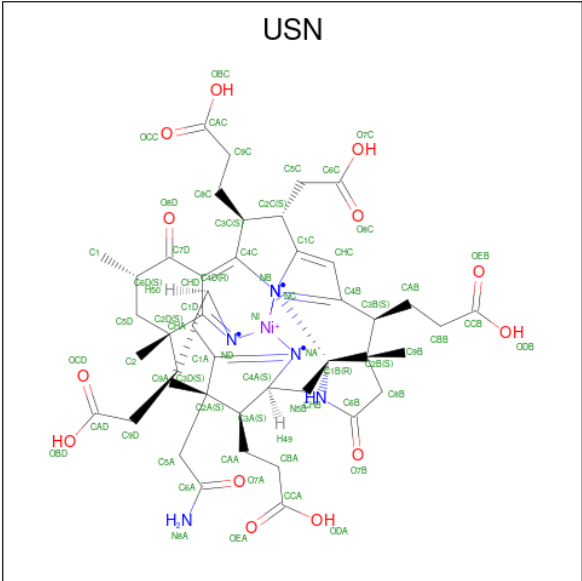
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl		
			2	2	0	0
8	C	1	Total	Cl		
			1	1	0	0
8	E	2	Total	Cl		
			2	2	0	0
8	F	1	Total	Cl		
			1	1	0	0

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	1
			8	4	1	3		
9	E	1	Total	C	N	O	0	1
			8	4	1	3		

- Molecule 10 is Dimethylated-F430 cofactor (CCD ID: USN) (formula: C₄₄H₅₅N₆NiO₁₃) (labeled as "Ligand of Interest" by depositor).



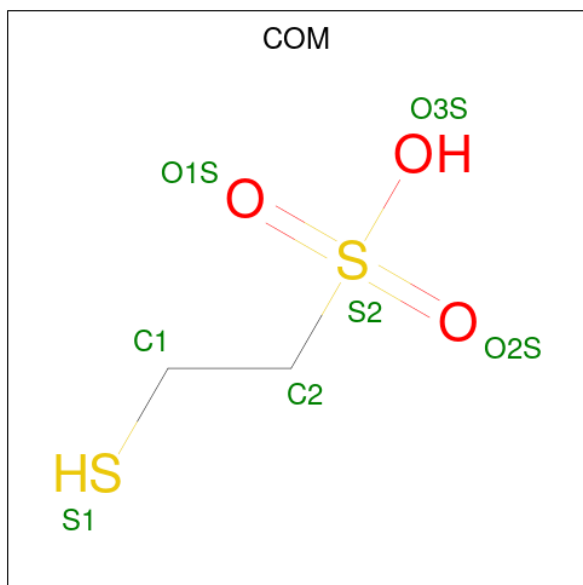
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	N	Ni	O	0	0
			64	44	6	1	13		

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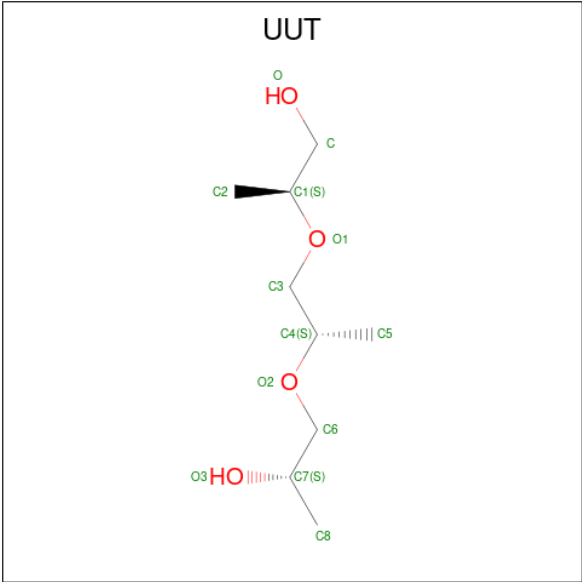
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	Ni	O	0	0
			64	44	6	1	13		

- Molecule 11 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
11	C	1	Total	C	O	S	0	0
			7	2	3	2		
11	F	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 12 is (2S)-2-{[(2S)-2-{[(2S)-2-hydroxypropyl]oxy}propyl]oxy}propan-1-ol (CCD ID: UUT) (formula: $C_9H_{20}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			13	9	4		
12	D	1	Total	C	O	0	0
			13	9	4		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	628	Total	O	0	63
			628	628		
13	B	574	Total	O	0	96
			574	574		
13	C	345	Total	O	0	26
			345	345		
13	D	642	Total	O	0	84
			642	642		
13	E	555	Total	O	0	75
			555	555		
13	F	342	Total	O	0	47
			342	342		

3 Residue-property plots

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: Ethyl-Coenzyme M reductase alpha subunit



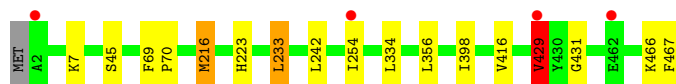
- Molecule 1: Ethyl-Coenzyme M reductase alpha subunit



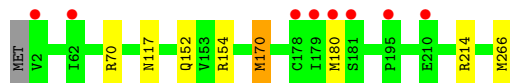
- Molecule 2: Ethyl-Coenzyme M reductase beta subunit



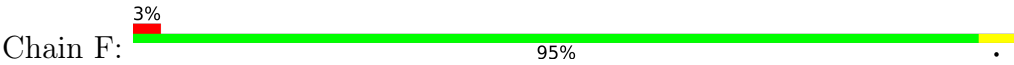
- Molecule 2: Ethyl-Coenzyme M reductase beta subunit



- Molecule 3: Ethyl-Coenzyme M reductase gamma subunit



- Molecule 3: Ethyl-Coenzyme M reductase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.74Å 146.93Å 113.13Å 90.00° 106.98° 90.00°	Depositor
Resolution (Å)	39.76 – 0.99 39.76 – 0.99	Depositor EDS
% Data completeness (in resolution range)	73.4 (39.76-0.99) 72.8 (39.76-0.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 0.99Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.112 , 0.128 0.128 , 0.141	Depositor DCC
R_{free} test set	52848 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	6.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	25172	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MN, CL, MGN, I2M, USN, AGM, HIC, GOL, COM, UUT, K, SMC, TRS, MHS, GL3, TP7

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	0.41	0/4950	0.68	2/6681 (0.0%)
1	D	0.41	0/4989	0.67	0/6729
2	B	0.40	0/3847	0.64	1/5212 (0.0%)
2	E	0.46	2/3875 (0.1%)	0.68	6/5250 (0.1%)
3	C	0.45	2/2368 (0.1%)	0.66	0/3190
3	F	0.47	0/2374	0.74	0/3201
All	All	0.43	4/22403 (0.0%)	0.67	9/30263 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	E	0	2
3	C	0	1
3	F	0	4
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	170[A]	MET	C-O	5.94	1.31	1.23
3	C	170[B]	MET	C-O	5.94	1.31	1.23
2	E	45[A]	SER	N-CA	5.45	1.52	1.46
2	E	45[B]	SER	N-CA	5.45	1.52	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229[A]	GLN	N-CA-C	5.55	117.77	111.11
1	A	229[B]	GLN	N-CA-C	5.55	117.77	111.11
2	B	69	PHE	CA-CB-CG	5.50	119.30	113.80
2	E	69	PHE	CA-CB-CG	5.46	119.26	113.80
2	E	429[A]	VAL	N-CA-C	-5.38	107.57	113.43

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	ARG	Sidechain
3	C	180[A]	MET	Mainchain
1	D	304	ARG	Sidechain
2	E	429[A]	VAL	Mainchain
2	E	429[B]	VAL	Mainchain

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	4862	0	4670	12	0
1	D	4879	0	4732	15	0
2	B	3737	0	3724	12	0
2	E	3731	0	3763	9	0
3	C	2299	0	2280	5	0
3	F	2317	0	2264	8	0
4	A	6	0	8	0	0
4	D	6	0	8	0	0
4	E	12	0	16	1	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1	0	0	0	0
9	B	8	0	12	0	0
9	E	8	0	12	0	0
10	C	64	0	0	0	0
10	D	64	0	0	0	0
11	C	7	0	5	0	0
11	F	7	0	4	0	0
12	C	13	0	0	0	0
12	D	13	0	0	0	0
13	A	628	0	0	0	0
13	B	574	0	0	2	0
13	C	345	0	0	1	0
13	D	642	0	0	2	0
13	E	555	0	0	3	0
13	F	342	0	0	0	0
All	All	25172	0	21536	59	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 59 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433[A]:GLU:H	2:B:433[A]:GLU:CD	2.01	0.66
3:C:152:GLN:HE21	3:C:154:ARG:HH21	1.52	0.58
3:C:152:GLN:NE2	3:C:154:ARG:HH21	2.05	0.55
2:E:466[A]:LYS:HG2	2:E:467:PHE:CE1	2.43	0.53
1:A:145:ILE:HG23	2:E:429[A]:VAL:HG11	1.91	0.51

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	614/595 (103%)	597 (97%)	15 (2%)	2 (0%)	36	12
1	D	618/595 (104%)	601 (97%)	15 (2%)	2 (0%)	36	12
2	B	497/467 (106%)	487 (98%)	10 (2%)	0	100	100
2	E	501/467 (107%)	495 (99%)	6 (1%)	0	100	100
3	C	285/266 (107%)	280 (98%)	5 (2%)	0	100	100
3	F	287/266 (108%)	280 (98%)	7 (2%)	0	100	100
All	All	2802/2656 (106%)	2740 (98%)	58 (2%)	4 (0%)	48	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	252[A]	SER
1	D	252[B]	SER
1	A	252[A]	SER
1	A	252[B]	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	499/470 (106%)	487 (98%)	12 (2%)	43	9
1	D	502/470 (107%)	498 (99%)	4 (1%)	73	38
2	B	396/364 (109%)	391 (99%)	5 (1%)	61	23
2	E	400/364 (110%)	393 (98%)	7 (2%)	51	15
3	C	258/236 (109%)	256 (99%)	2 (1%)	73	38
3	F	259/236 (110%)	254 (98%)	5 (2%)	50	14
All	All	2314/2140 (108%)	2279 (98%)	35 (2%)	68	19

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	254[A]	ILE

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Mol	Chain	Res	Type
2	E	254[B]	ILE
3	F	117	ASN
2	B	216[A]	MET
1	A	323[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	375	ASN
1	D	494	GLN
1	D	450	GLN
2	E	134	ASN
1	A	450	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	D	305	1	10,11,12	0.50	0	7,13,15	0.60	0
1	MHS	A	291	1	10,11,12	1.04	0	5,14,16	4.07	2 (40%)
1	GL3	D	490	1	2,3,4	3.25	1 (50%)	1,2,4	0.31	0
1	MGN	A	445	1	6,9,10	0.67	0	7,12,14	0.42	0
1	SMC	D	354	1	5,6,7	0.58	0	3,6,8	0.85	0
1	AGM	A	305	1	10,11,12	0.49	0	7,13,15	0.59	0
1	SMC	A	354	1	5,6,7	0.60	0	3,6,8	0.67	0
1	MGN	D	445	1	6,9,10	0.67	0	7,12,14	0.24	0
1	HIC	A	491	1	10,11,12	1.08	0	9,14,16	3.09	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	I2M	A	377	1	7,8,9	1.12	1 (14%)	6,11,13	1.18	1 (16%)
1	HIC	D	491	1	10,11,12	0.92	0	9,14,16	2.96	2 (22%)
1	I2M	D	377	1	7,8,9	0.80	0	6,11,13	1.10	0
1	MHS	D	291	1	10,11,12	0.96	0	5,14,16	4.30	2 (40%)
1	GL3	A	490	1	2,3,4	2.49	1 (50%)	1,2,4	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	D	305	1	-	2/10/11/13	-
1	MHS	A	291	1	-	0/5/6/8	0/1/1/1
1	GL3	D	490	1	-	0/1/1/2	-
1	MGN	A	445	1	-	0/7/9/12	-
1	SMC	D	354	1	-	0/3/5/7	-
1	AGM	A	305	1	-	2/10/11/13	-
1	SMC	A	354	1	-	0/3/5/7	-
1	MGN	D	445	1	-	0/7/9/12	-
1	HIC	A	491	1	-	2/5/6/8	0/1/1/1
1	I2M	A	377	1	-	0/7/11/13	-
1	HIC	D	491	1	-	2/5/6/8	0/1/1/1
1	I2M	D	377	1	-	0/7/11/13	-
1	MHS	D	291	1	-	0/5/6/8	0/1/1/1
1	GL3	A	490	1	-	0/1/1/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	490	GL3	C-S	-4.59	1.61	1.80
1	A	490	GL3	C-S	-3.52	1.66	1.80
1	A	377	I2M	CB-CA	-2.53	1.53	1.57

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	MHS	ND1-CE1-NE2	-9.08	107.54	112.94
1	A	291	MHS	ND1-CE1-NE2	-8.63	107.80	112.94
1	D	491	HIC	NE2-CE1-ND1	-7.90	109.64	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	HIC	NE2-CE1-ND1	-7.64	109.74	112.66
1	A	491	HIC	CD2-NE2-CE1	4.89	108.64	106.71

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	491	HIC	CA-CB-CG-CD2
1	A	491	HIC	CA-CB-CG-CD2
1	A	491	HIC	CA-CB-CG-ND1
1	D	491	HIC	CA-CB-CG-ND1
1	D	305	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	490	GL3	1	0
1	A	491	HIC	1	0
1	D	491	HIC	1	0
1	A	490	GL3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 11 are monoatomic - leaving 14 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	GOL	E	505[A]	-	5,5,5	0.17	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	UUT	D	1105	-	12,12,12	0.64	0	14,14,14	0.97	1 (7%)
5	TP7	D	1102	-	19,20,20	0.66	0	24,26,26	0.69	0
11	COM	C	302	10	6,6,6	0.81	0	8,8,8	0.58	0
12	UUT	C	305	-	12,12,12	0.68	0	14,14,14	1.16	1 (7%)
9	TRS	B	503[A]	-	7,7,7	0.28	0	9,9,9	0.52	0
10	USN	D	1101	11	63,73,73	2.26	10 (15%)	76,123,123	1.21	7 (9%)
5	TP7	A	602	-	19,20,20	0.74	0	24,26,26	0.82	1 (4%)
10	USN	C	301	11	63,73,73	2.17	7 (11%)	76,123,123	1.04	6 (7%)
11	COM	F	401	10	6,6,6	0.93	0	8,8,8	0.66	0
9	TRS	E	501[A]	-	7,7,7	0.33	0	9,9,9	0.37	0
4	GOL	E	502	-	5,5,5	0.28	0	5,5,5	0.62	0
4	GOL	D	1103	-	5,5,5	0.09	0	5,5,5	0.31	0
4	GOL	A	601	-	5,5,5	0.17	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	505[A]	-	-	4/4/4/4	-
12	UUT	D	1105	-	-	2/12/12/12	-
5	TP7	D	1102	-	-	0/24/24/24	-
11	COM	C	302	10	-	0/4/4/4	-
12	UUT	C	305	-	-	2/12/12/12	-
9	TRS	B	503[A]	-	-	5/9/9/9	-
10	USN	D	1101	11	1/1/31/33	2/28/193/193	-
10	USN	C	301	11	1/1/31/33	2/28/193/193	-
5	TP7	A	602	-	-	0/24/24/24	-
11	COM	F	401	10	-	0/4/4/4	-
9	TRS	E	501[A]	-	-	1/9/9/9	-
4	GOL	E	502	-	-	0/4/4/4	-
4	GOL	D	1103	-	-	3/4/4/4	-
4	GOL	A	601	-	-	3/4/4/4	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	301	USN	NI-NA	10.50	2.14	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1101	USN	NI-NA	10.01	2.13	1.89
10	D	1101	USN	NI-NB	9.52	2.12	1.89
10	C	301	USN	NI-NB	8.43	2.09	1.89
10	D	1101	USN	NI-ND	7.01	2.06	1.89

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1101	USN	C2C-C5C-C6C	-3.74	106.94	113.95
10	C	301	USN	C2B-C1B-NB	3.58	107.17	101.86
12	C	305	UUT	C3-O1-C1	3.28	119.88	115.05
10	C	301	USN	C2C-C5C-C6C	-3.06	108.22	113.95
10	D	1101	USN	C2B-C1B-NB	3.04	106.37	101.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	C	301	USN	NC
10	D	1101	USN	NC

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	505[A]	GOL	O1-C1-C2-C3
4	E	505[A]	GOL	C1-C2-C3-O3
9	B	503[A]	TRS	N-C-C1-O1
9	B	503[A]	TRS	C1-C-C2-O2
9	B	503[A]	TRS	C3-C-C2-O2

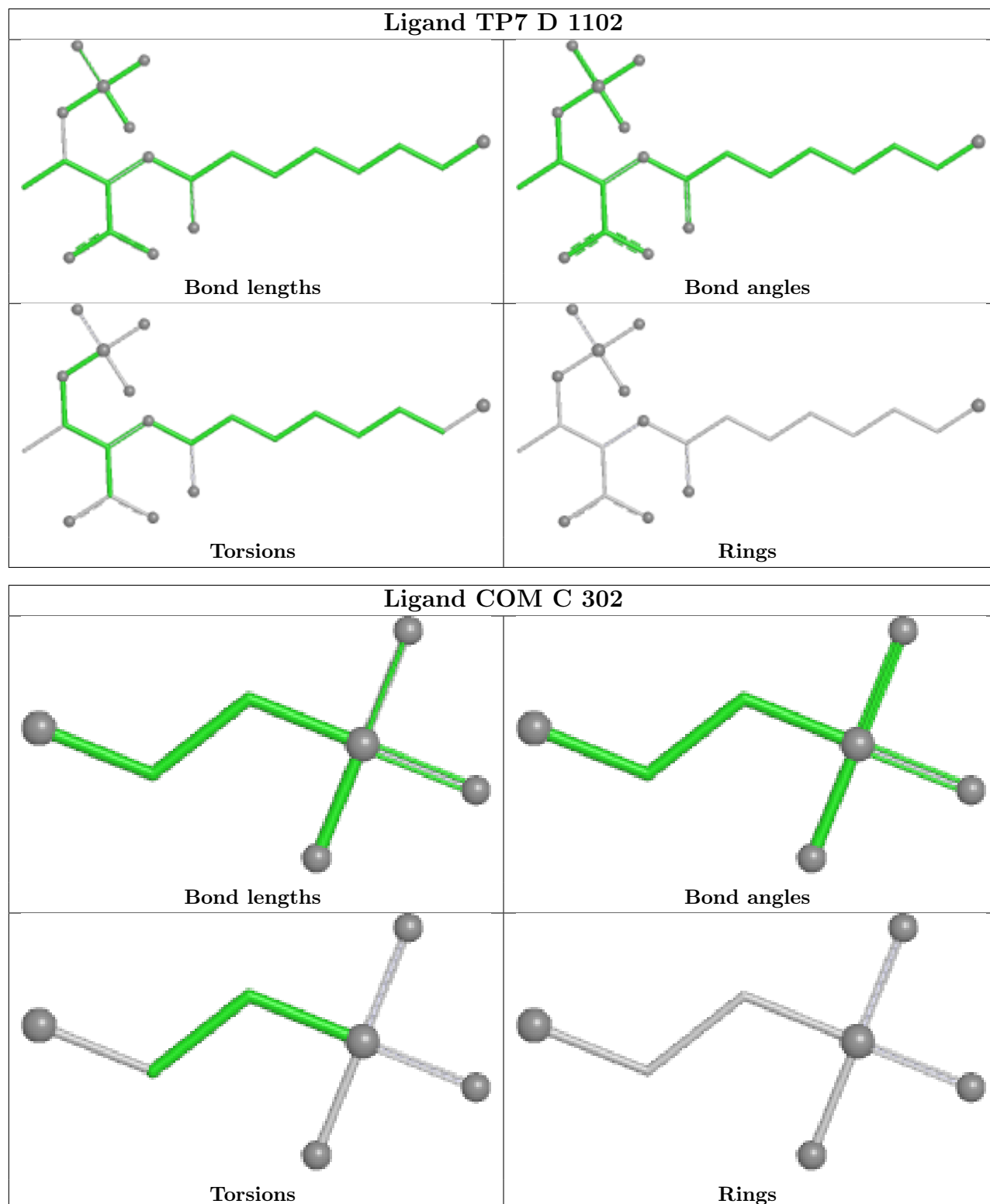
There are no ring outliers.

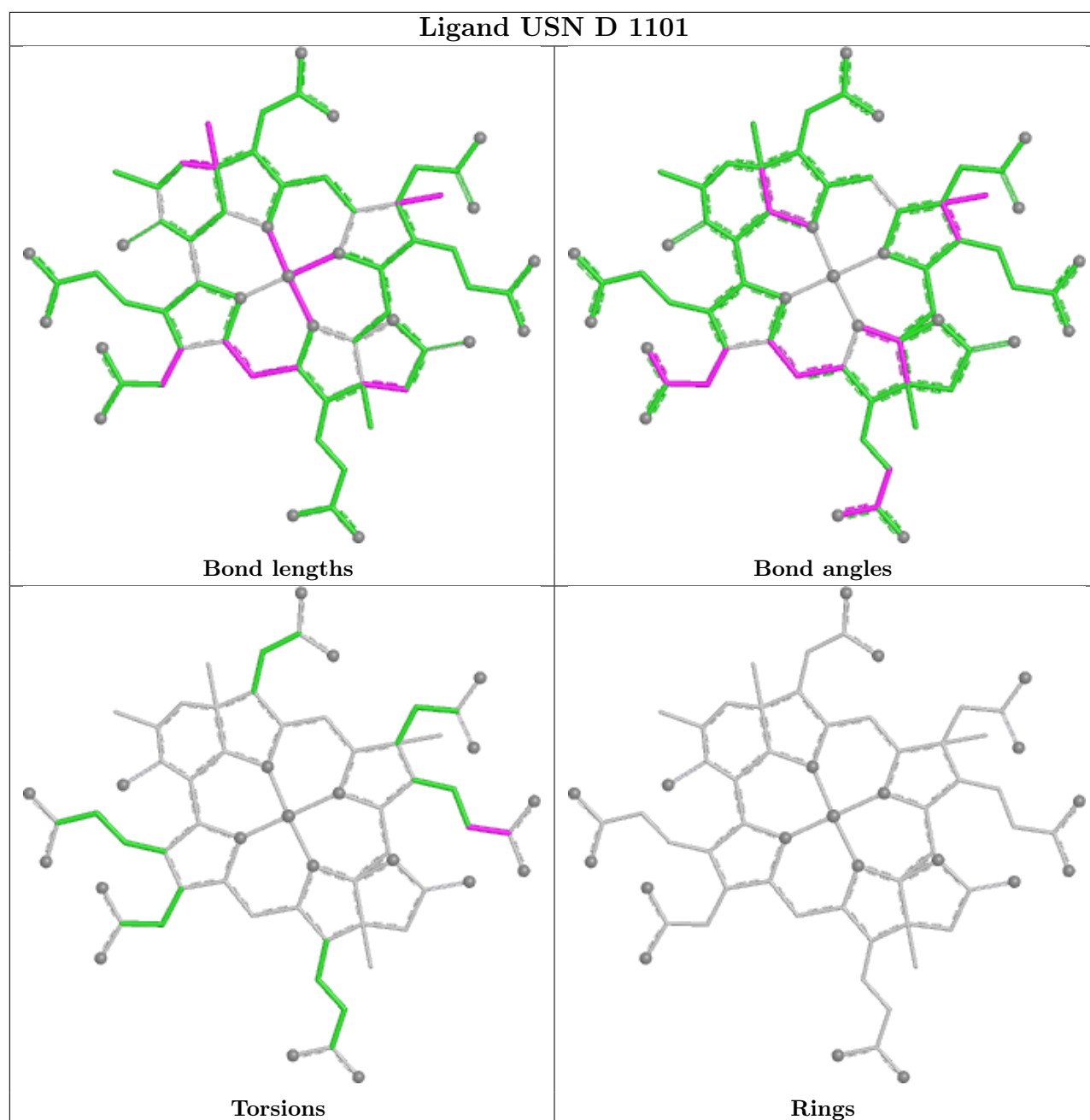
1 monomer is involved in 1 short contact:

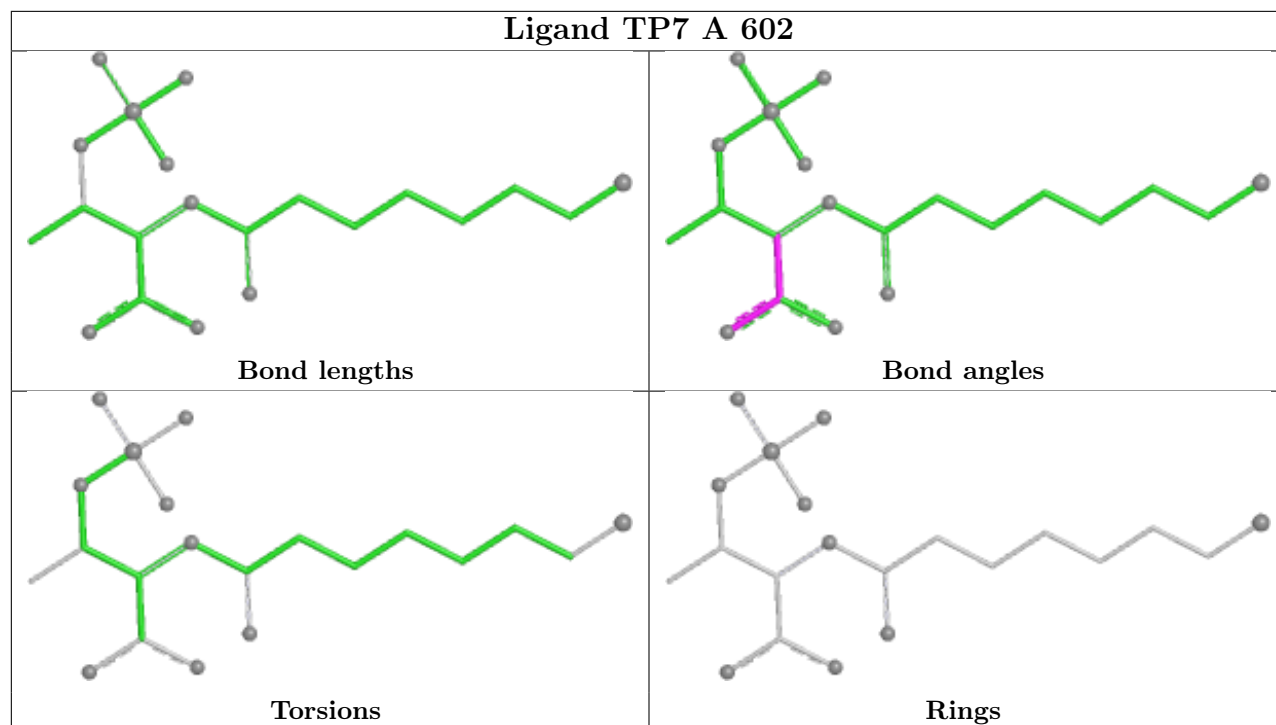
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	502	GOL	1	0

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

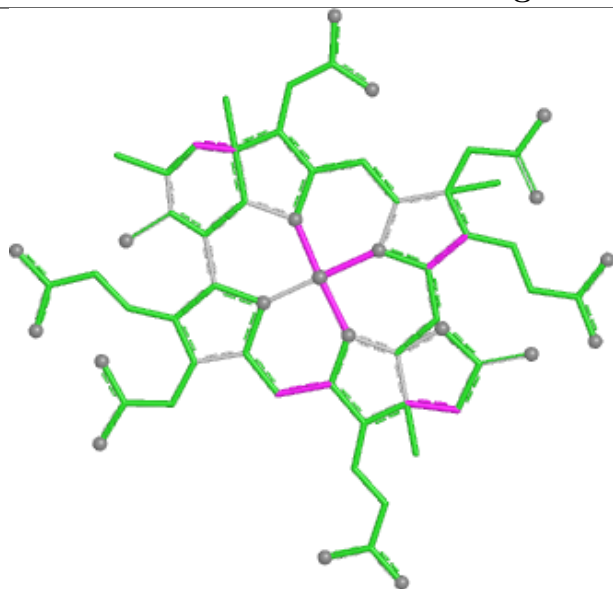
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



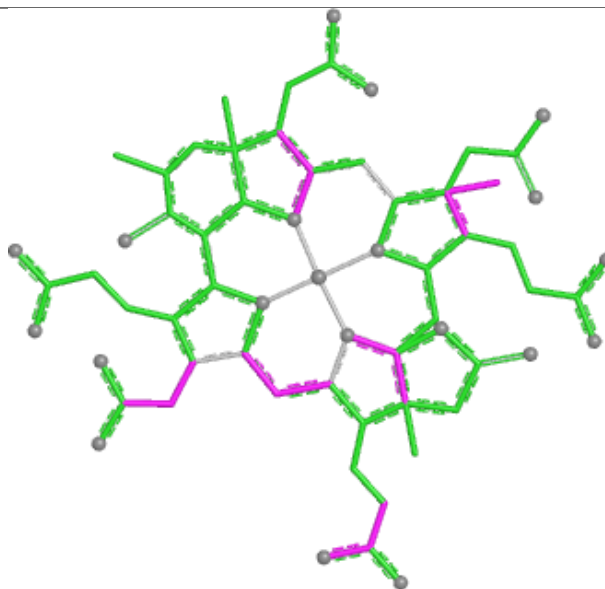




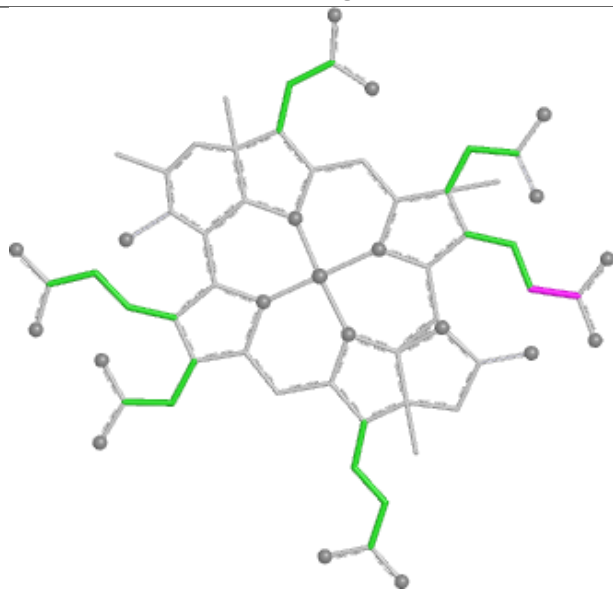
Ligand USN C 301



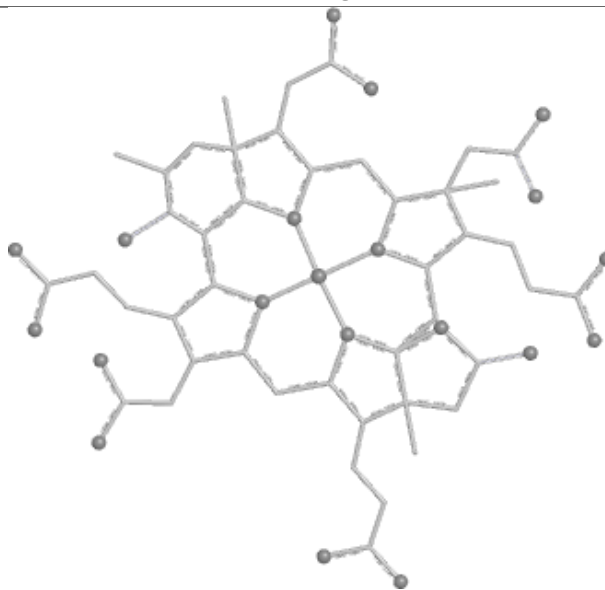
Bond lengths



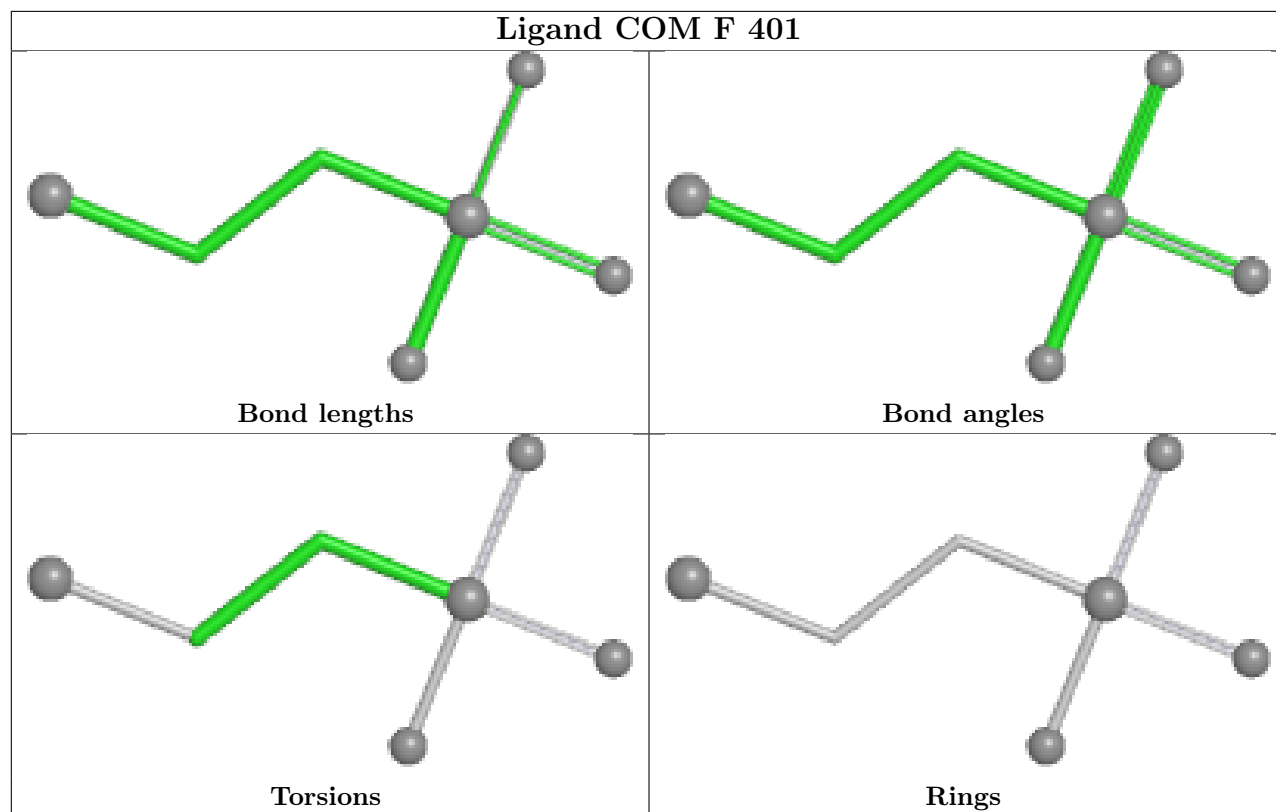
Bond angles



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, 95th 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	584/595 (98%)	-0.49	3 (0%) 87 90	3, 7, 14, 31	33 (5%)
1	D	586/595 (98%)	-0.54	6 (1%) 79 84	2, 6, 13, 35	35 (5%)
2	B	466/467 (99%)	-0.30	10 (2%) 63 70	3, 8, 17, 32	33 (7%)
2	E	466/467 (99%)	-0.42	4 (0%) 81 85	3, 7, 14, 24	37 (7%)
3	C	265/266 (99%)	0.06	8 (3%) 52 59	5, 10, 20, 30	23 (8%)
3	F	265/266 (99%)	-0.10	8 (3%) 52 59	4, 8, 17, 28	24 (9%)
All	All	2632/2656 (99%)	-0.36	39 (1%) 72 78	2, 7, 16, 35	185 (7%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	6.1
3	C	2	VAL	5.5
3	F	2	VAL	5.4
1	D	3	LYS	3.9
1	D	4	TYR	3.8

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, 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
1	MHS	A	291	11/12	0.99	0.04	4,5,6,6	0
1	MHS	D	291	11/12	0.99	0.03	5,5,6,7	0
1	AGM	A	305	12/13	0.99	0.03	4,5,5,6	0
1	AGM	D	305	12/13	0.99	0.02	4,5,5,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	I2M	A	377	9/10	0.99	0.04	5,5,8,9	0
1	I2M	D	377	9/10	0.99	0.04	4,4,7,9	0
1	MGN	A	445	10/11	0.99	0.03	5,6,6,6	0
1	MGN	D	445	10/11	0.99	0.02	4,4,4,5	0
1	HIC	A	491	11/12	0.99	0.03	4,5,5,5	0
1	HIC	D	491	11/12	0.99	0.03	3,4,4,4	0
1	GL3	A	490	4/5	1.00	0.02	4,5,5,5	0
1	GL3	D	490	4/5	1.00	0.03	3,3,4,4	0
1	SMC	A	354	7/8	1.00	0.03	4,5,6,8	0
1	SMC	D	354	7/8	1.00	0.03	4,4,5,7	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, 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($\text{\AA}^2$)	Q<0.9
4	GOL	D	1103	6/6	0.64	0.20	39,40,40,40	0
4	GOL	A	601	6/6	0.68	0.17	38,39,39,39	0
4	GOL	E	505[A]	6/6	0.73	0.32	14,17,18,19	6
4	GOL	E	502	6/6	0.75	0.18	35,36,36,36	0
9	TRS	E	501[A]	8/8	0.87	0.14	10,15,16,18	8
12	UUT	C	305	13/13	0.89	0.14	14,22,28,29	0
9	TRS	B	503[A]	8/8	0.92	0.09	12,13,14,14	8
12	UUT	D	1105	13/13	0.93	0.12	11,20,28,29	0
7	K	A	604	1/1	0.98	0.14	19,19,19,19	0
7	K	A	605[A]	1/1	0.98	0.12	14,14,14,14	1
8	CL	C	303	1/1	0.98	0.08	31,31,31,31	0
8	CL	F	402	1/1	0.98	0.10	31,31,31,31	0
8	CL	E	504	1/1	0.99	0.03	8,8,8,8	1
5	TP7	D	1102	21/21	0.99	0.04	4,5,6,7	0
5	TP7	A	602	21/21	0.99	0.04	5,6,7,7	0
7	K	C	304	1/1	1.00	0.13	15,15,15,15	0
7	K	D	1104[A]	1/1	1.00	0.06	12,12,12,12	1
8	CL	B	501	1/1	1.00	0.06	11,11,11,11	0

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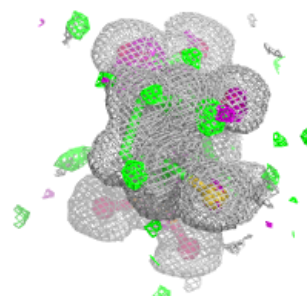
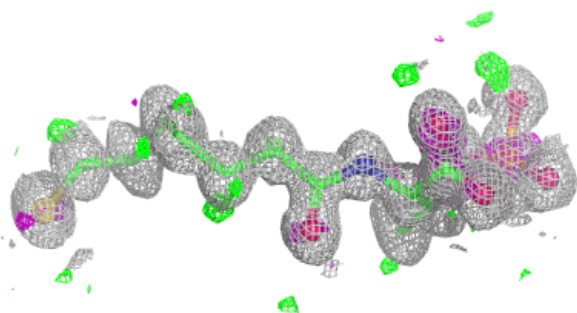
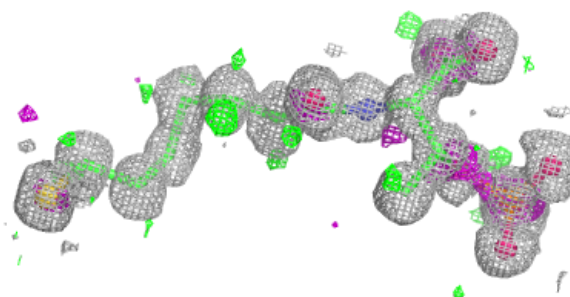
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	B	502	1/1	1.00	0.03	8,8,8,8	1
10	USN	C	301	64/64	1.00	0.03	4,5,8,9	0
10	USN	D	1101	64/64	1.00	0.03	3,4,6,7	0
11	COM	C	302	7/7	1.00	0.03	5,6,6,7	0
11	COM	F	401	7/7	1.00	0.03	4,4,6,6	0
6	MN	A	603	1/1	1.00	0.04	8,8,8,8	0
8	CL	E	503	1/1	1.00	0.06	10,10,10,10	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.

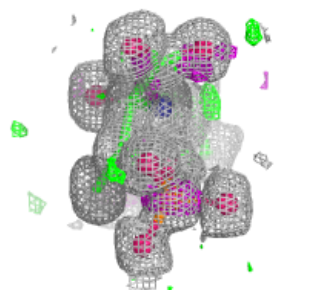
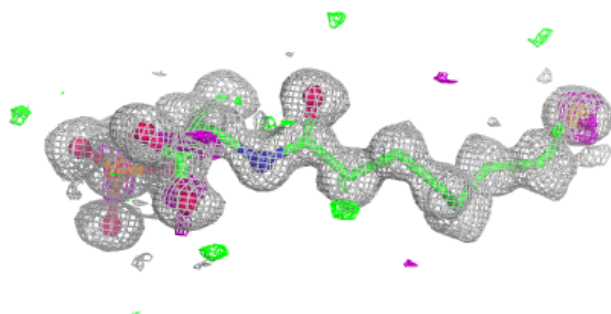
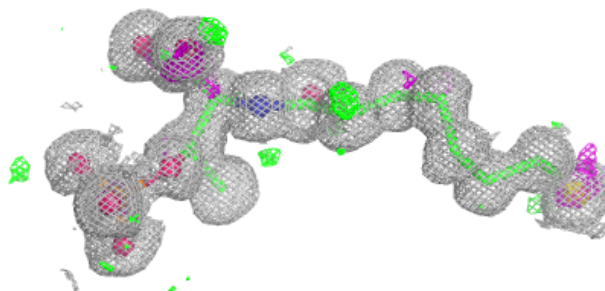
Electron density around TP7 D 1102:

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



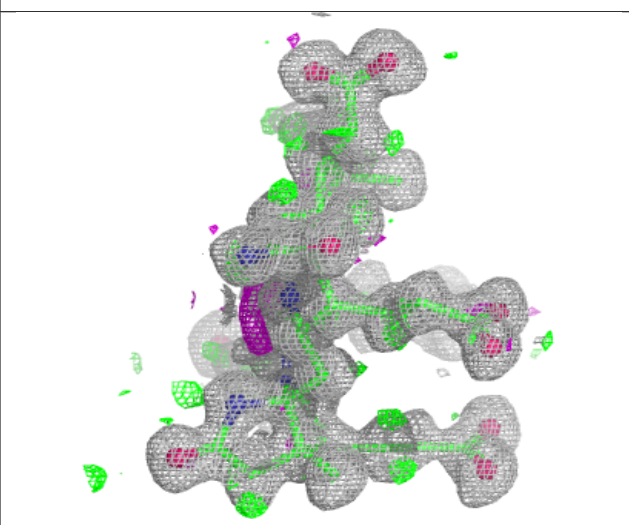
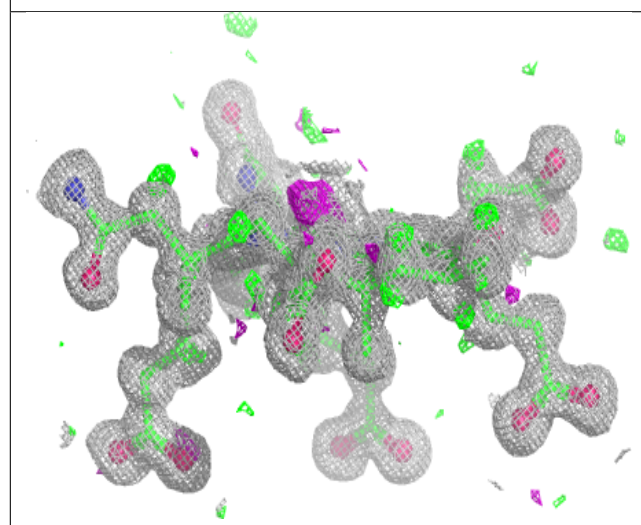
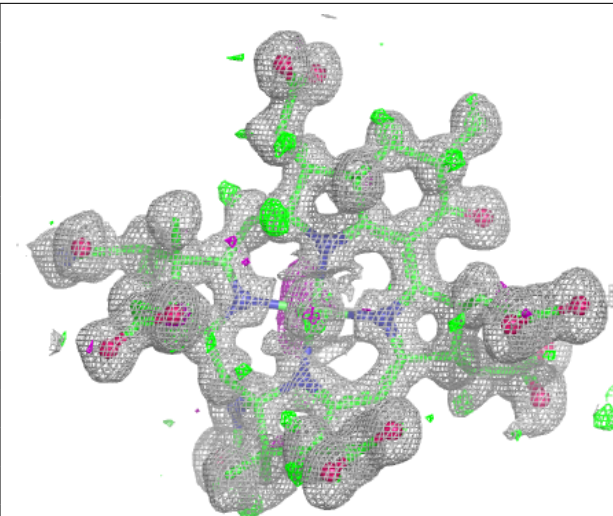
Electron density around TP7 A 602:

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



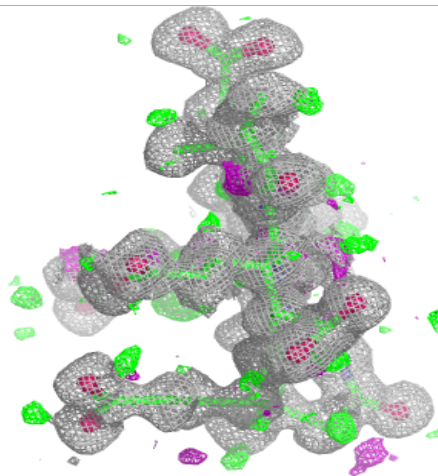
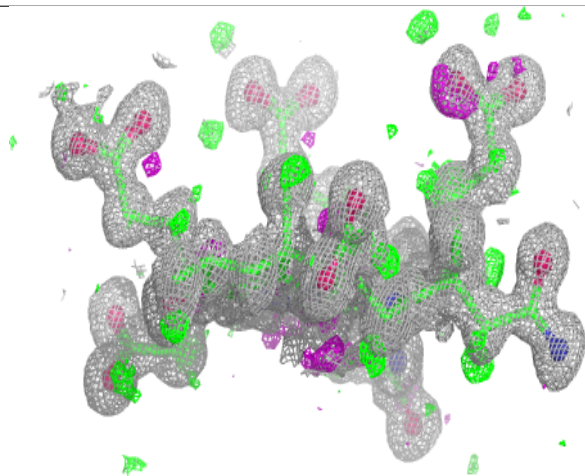
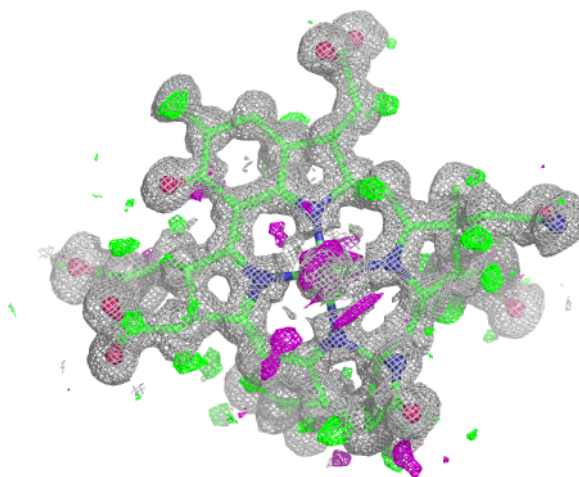
Electron density around USN C 301:

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



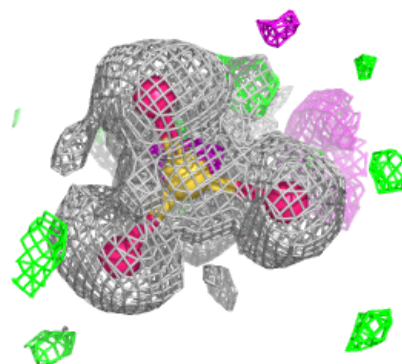
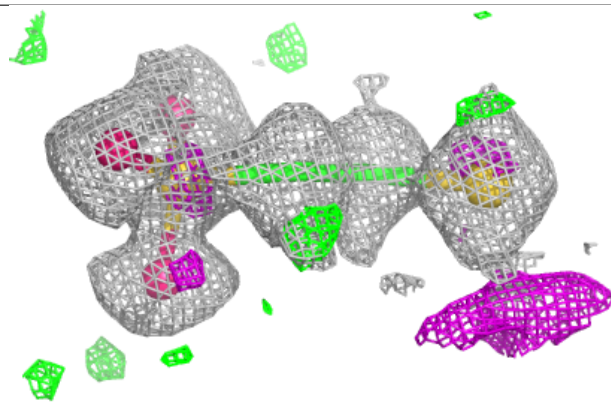
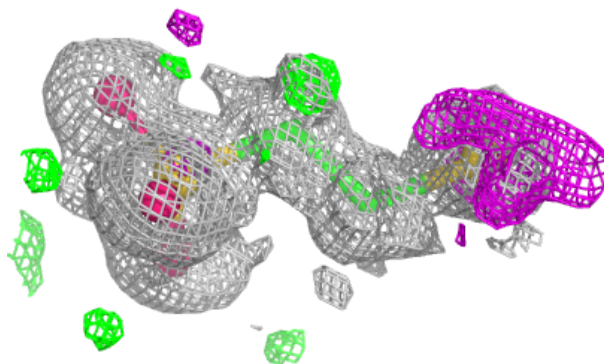
Electron density around USN D 1101:

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

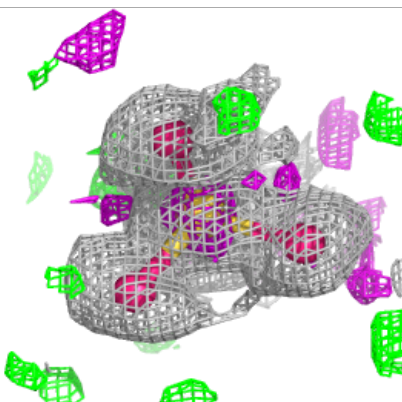
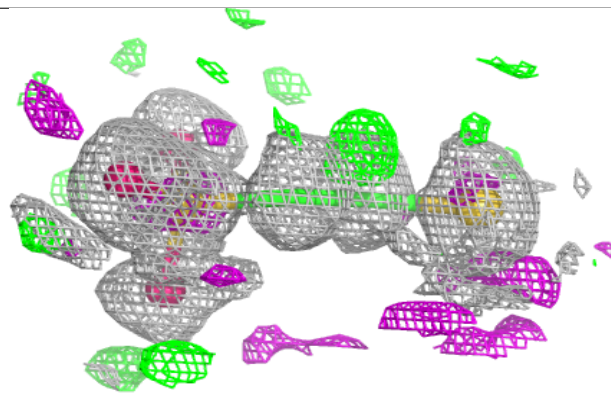
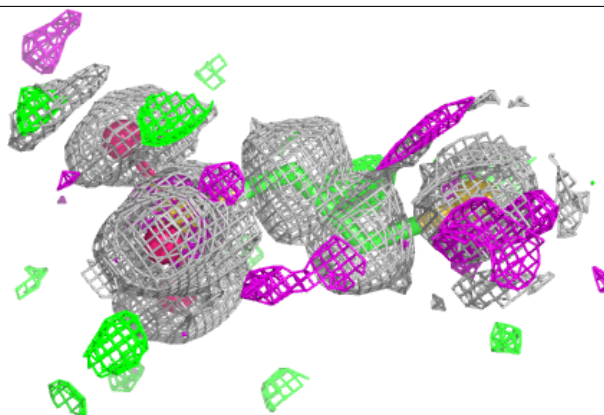


Electron density around COM C 302:

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

**Electron density around COM F 401:**

$2mF_o-DF_c$ (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.